

Representative statistical ensembles for Bose systems with broken gauge symmetry

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Abstract

Bose-condensed systems with broken global gauge symmetry are considered. The description of these systems, as has been shown by Hohenberg and Martin, possesses an internal inconsistency, resulting in either nonconserving theories or yielding an unphysical gap in the spectrum. The general notion of representative statistical ensembles is formulated for arbitrary statistical systems, equilibrium or not. The principal idea of this notion is the necessity of taking into account all imposed conditions that uniquely define the given statistical system. Employing such a representative ensemble for Bose-condensed systems removes all paradoxes, yielding a completely self-consistent theory, both conserving and gapless in any approximation. This is illustrated for an equilibrium uniform Bose system.

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1 Introduction and Analysis of Problem

The appearance of Bose-Einstein condensate in a Bose system is usually associated with the breaking of the global gauge symmetry, which is commonly realized by means of the Bogolubov shift in the field operators [1–4]. The idea of symmetry breaking is in line with the general understanding that phase transitions of different nature are accompanied by some symmetry changes. In theoretical description, there exist several ways of symmetry breaking (see review article [5]). The most known is the Bogolubov method of quasiaverages, when the symmetry of the Hamiltonian is disturbed by infinitesimal sources [4]. For breaking the global gauge symmetry, the latter technique is not always convenient, while the Bogolubov shift is a simple and sufficient condition for the symmetry breaking [6].

When the global gauge symmetry is broken, then the description of Bose systems, based on the standard grand canonical ensemble, encounters a dilemma, first discussed by Hohenberg and Martin [7], who emphasized that this description results in either nonconserving theories or yields an unphysical gap in the spectrum of particles. In nonconserving theories, local conservation laws are not valid, which, at the same time, is connected with inconsistencies in thermodynamics.

The Hohenberg-Martin dilemma of conserving versus gapless theories is usually illustrated by considering some approximate schemes [7], for instance, a kind of mean-field approximations. The origin of this dilemma can be explained as follows.

Bose-Einstein condensation implies the macroscopic occupation of the ground-state energy level, when the number of condensed particles N_0 is such that the condensate fraction N_0/N is nonzero in the thermodynamic limit. The total number of particles in the system, $N = N_0 + N_1$, becomes a sum of the condensed-particle number N_0 and the number N_1 of uncondensed particles. According to Bogolubov [1–4], the number of condensed particles N_0 is such that it provides thermodynamic stability for the system, minimizing the thermodynamic potential. At the same time, $N_0 = N - N_1$, where $N_1 = N_1(\mu, T, \rho)$ is a function of the chemical potential μ , temperature T , and density $\rho \equiv N/V$, with V being the system volume. Hence, $N_0 = N_0(\mu, T, \rho)$ is a function of the same variables. Conversely, the chemical potential $\mu = \mu(T, \rho)$ is a function of T and ρ . Thus, the condition of the stability, realized as the minimization of the thermodynamic potential, defines the chemical potential μ . It is important to emphasize that this procedure of minimization does not depend on approximations, but is generally valid, as was strictly proved by Ginibre [8].

From another side, the particle spectrum, under the broken gauge symmetry, has to be gapless. This is, actually, the condition for the existence of stable Bose-Einstein condensate. Since, if there would be a gap in the spectrum, there could be no macroscopic occupation of a single ground-state level. Hugenholtz and Pines [9] showed that the chemical potential $\mu = \Sigma_{11}(0, 0) - \Sigma_{12}(0, 0)$ is expressed through the self-energies $\Sigma_{\alpha\beta}(\mathbf{k}, \omega)$, and this relation makes the spectrum gapless for any Bose system. As far as the self-energies $\Sigma_{\alpha\beta}(0, 0)$ are the functions of T and ρ , the Hugenholtz-Pines relation defines the chemical potential $\mu = \mu(T, \rho)$.

In this way, the condition of thermodynamic stability, in the frame of the Bogolubov-Ginibre minimization procedure, defines a chemical potential that we shall denote as μ_{BG} . At the same time, the existence of a gapless spectrum, connected to the Hugenholtz-Pines relation, also defines a chemical potential, which may be denoted as μ_{HP} . These chemical potentials, found in two different ways do not necessarily coincide, and, generally, they

are different: $\mu_{BG} \neq \mu_{HP}$. Therefore, if one accepts as the system chemical potential the Bogolubov-Ginibre value μ_{BG} , providing thermodynamic stability, then one acquires an unphysical gap in the spectrum, proportional to the difference $|\mu_{HP} - \mu_{BG}|^{1/2}$. Conversely, accepting as the chemical potential the Hugenholtz-Pines form μ_{HP} , one gets a nonconserving theory with incorrect thermodynamics, since the stability condition does not hold. This is the origin of the Hohenberg-Martin dilemma of conserving versus gapless theories [7].

In any case, the fact that $\mu_{BG} \neq \mu_{HP}$ makes the system unstable and its description not self-consistent. This problem does not arise only in the limit of asymptotically weak interactions, when the Bogolubov weakly-nonideal gas approximation is applicable [1,2]. In this limit, μ_{BG} and μ_{HP} asymptotically coincide. However, in any higher approximation one has $\mu_{BG} \neq \mu_{HP}$.

For practical applications, one usually does the following. When one is interested solely in the system dynamics, but not in its spectrum, one derives the equations from a variational principle, which guarantees the validity of conservation laws [10,11]. For an equilibrium system, this is equivalent to the Bogolubov-Ginibre variational procedure. And, when one studies only the system spectrum, one accepts the Hugenholtz-Pines relation, forgetting about inconsistent thermodynamics and instability. Clearly, such palliative ways are not satisfactory. The principal problem remains how to make the general theory both conserving as well as gapless.

There have been several attempts to cure the problem, which could be classified into three groups:

The most often used trick is the omission of anomalous averages. As is clear, this is a rather unjustified way, since, as soon as the global gauge symmetry is broken, the anomalous averages do exist and are not zero. One, sometimes, ascribes this trick to Popov, calling it the "Popov approximation". However, it is sufficient to look attentively at the original works by Popov [12–14], which are usually cited in this respect, in order to realize that he has never suggested anything like that. He considered the properties of a Bose gas in the vicinity of the critical temperature T_c , honestly calculating all terms, normal and anomalous. When temperature tends to T_c , the condensate density tends to zero together with the anomalous averages. Actually, both these quantities, the condensate density and the anomalous averages are the order parameters, appearing together in the broken-symmetry phase, and disappearing also together, when the symmetry is getting restored at the critical temperature. Contrary to this, the normal average, that is, the density of uncondensed particles, increases when approaching the critical temperature, reaching at T_c the total system density. This is why at the close vicinity of T_c , the anomalous averages become, without any special assumptions, smaller than the normal ones. However at low temperatures $T \ll T_c$, the anomalous averages not merely can be of the order of the normal averages, but can even be much larger than the latter, as direct calculations show [15]. Moreover, omitting the anomalous averages makes the system principally unstable [15,16]. Thus, this trick neither has anything to do with Popov nor can be accepted as a reasonable approximation at low temperatures. Additionally, if one would wish to ascribe a name to this trick, one should know that the first person, who really suggested and used it, was Shohno [17]. And this was known in literature as the Shohno model. The word "model" is appropriate here, since this is, actually, just a model, but not a justified approximation. For example, Reatto and Straley [18] used the term "Shohno model" and studied its properties.

Another way of removing the gap in the spectrum is to calculate the chemical potential

and self energy in different approximations. Then one defines the chemical potential from the thermodynamic stability condition in one approximation, but for calculating the self-energy, one invokes a higher-order approximation, so that to cancel the gap. The additional higher-order terms can be motivated by Bethe-Salpeter or scattering-matrix approximations [19,20]. This way is what was called by Bogolubov [4] the mismatch of approximations. Bogolubov already mentioned [4] that such a mismatch can really influence the appearance or disappearance of the spectrum gap, but renders the theory not self-consistent and the system unstable.

One can also kill the spectrum gap by adding to the self-energy phenomenological terms, such that to cancel the gap [21–23]. This way is, clearly, equivalent to the previous one, since changing the self-energy by invoking some higher-order approximations is not unique and, hence, is also phenomenological.

As is evident, all these ways, attempting to cure the problem, are based on a kind of the mismatch of approximations and, as a result, they have the same common defects:

(i) They are not uniquely defined since there exists an infinite number of particular tricks for removing the spectrum gap. So, the ambiguity remains [23].

(ii) They are not self-consistent, involving in this or that way the mismatch of approximations [4].

(iii) They, as a rule, correspond to an unstable system, either with a not minimal thermodynamic potential or with a divergent susceptibility [15,16].

(iv) The order of the condensation transitions changes, resulting in a first-order phase transition, instead of the correct second-order one. This happens because of the internal inconsistencies in the description. The disruption of the phase-transition order is a common feature of inconsistent approximations, which either do not satisfy the stability conditions or possess a spectrum gap [18,21–23]. This was already noticed in the early works analysing the Hartree-Fock-Bogolubov approximation having a gap in the spectrum [18,24–27]. The generality of such a change of the phase-transition order from second to first in different mean-field approximations was emphasized in a detailed discussion by Baym and Grinstein [28] and recently by Kita [23]. As is clear, the thermodynamics of a system with a first-order phase transition is rather different from that of a system displaying a second-order transition. And in the vicinity of the critical point, the thermodynamics in these two cases differs drastically [23,28].

(v) Finally, the mismatch of approximations, by its own, is not a regular procedure. For each given approximation, it is necessary to invent special tricks, which, as is stressed above, are not uniquely defined, hence, ambiguous. There is no a general rule how to do this in a unique way for approximations of different order.

Thus, we have to conclude that the Hohenberg-Martin dilemma [7] remains unsolved. The methods, based on the mismatch of approximations, are not self-consistent, having several internal defects discussed above. In order that an effective theory be self-consistent, all dynamic and thermodynamic equations must be derived from the same Hamiltonian, or Lagrangian, and treated in one chosen approximation, without involving the approximation mismatch [29,30]. The most recent thorough discussion of the Hohenberg-Martin dilemma, with many citations, can be found in the review article by Andersen [31].

In the paper [6], the idea was advanced that the problem can be solved by employing a representative statistical ensemble. In Refs. [32,33], it was shown how to make the Hartree-Fock-Bogolubov (HFB) approximation for a dilute gas both conserving and gapless. The

aim of the present paper is to develop a general approach, independent of particular approximations, for the self-consistent treatment of arbitrary Bose systems with broken gauge symmetry and to demonstrate on the most general footing that the resulting theory is really completely self-consistent. The approach is based on the notion of representative statistical ensembles, whose general formulation is given in Sec. 2 for both equilibrium as well as nonequilibrium systems. This notion is specified in Sec. 3 for Bose systems with broken gauge symmetry. Thermodynamic self-consistency of the theory is emphasized in Sec. 4. Operator equations of motion are obtained in Sec. 5 for a Hamiltonian with an arbitrary interaction potential. Sec. 6 demonstrates that the local conservation laws are valid on the operator level, hence, being automatically satisfied for the related average quantities. The equation for the condensate wave function is derived and analyzed in Sec. 7 for an arbitrary Bose system. In Sec. 8 a uniform Bose system is considered and illustrated for the HFB approximation. The behaviour of the condensate and superfluid fractions is studied in Sec. 9. The equations for Green functions are presented in Sec. 10, where it is shown, by using the Bogolubov theorem [4], that the Hugenholtz-Pines relation follows, thus, proving the complete self-consistency of the developed approach. Sec. 11 is the conclusion.

Throughout the paper, the system of units is used, where the Planck and Boltzmann constants are set to unity, $\hbar = 1$, $k_B = 1$.

2 Representative Statistical Ensembles

The idea of representative statistical ensembles goes back to Gibbs [34], who mentioned that to prescribe a canonical distribution for a system may be not sufficient, but this distribution has to be complimented by those constraints and conditions that provide a correct representation of the considered statistical system. The term "representative ensembles" was used by ter Haar [35,36], who investigated the problem of a proper representation of equilibrium statistical systems. Equilibrium and quasiequilibrium representative ensembles were described in the review article [5]. In this section, we shall formulate the notion of representative statistical ensembles for both equilibrium and nonequilibrium systems.

Representative statistical ensembles for equilibrium systems are sometimes also termed as generalized Gibbs ensembles, subjective or conditional ensembles. Their mathematical construction is based on the conditional maximization of the Gibbs entropy, as was done by Janes [37,38]. This concept was also employed by Girardeau [39].

Let us start with equilibrium systems. An *equilibrium statistical ensemble*, by definition, is a pair $\{\mathcal{F}, \hat{\rho}\}$ of the space \mathcal{F} of microstates and a statistical operator $\hat{\rho}$. In order to correctly define the latter, it is necessary, according to Gibbs [34], to take into account all conditions and constraints, imposed on the system. Suppose, we have a set $\{\hat{C}_i\}$ of self-adjoint operators, defined on the space \mathcal{F} , which will be called condition operators. This is because these operators enter the *statistical conditions*

$$C_i = \langle \hat{C}_i \rangle = \text{Tr} \hat{\rho} \hat{C}_i, \quad (1)$$

which are necessary to take into account for correctly representing the considered system. The trace operation in Eq. (1) is over the given space \mathcal{F} , which can be defined as a Fock space. The first evident constraint is the normalization condition for the statistical operator,

$$1 = \langle \hat{1}_{\mathcal{F}} \rangle = \text{Tr} \hat{\rho}, \quad (2)$$

where $\hat{1}_{\mathcal{F}}$ is the unity operator in \mathcal{F} . The definition of the internal energy

$$E = \langle \hat{H} \rangle = \text{Tr} \hat{\rho} \hat{H} , \quad (3)$$

as the average of a Hamiltonian \hat{H} , is another standard statistical condition. But, in addition to constraints (2) and (3), there can exist any number of other statistical conditions (1). The conditional maximization of the Gibbs entropy

$$S \equiv -\text{Tr} \hat{\rho} \ln \hat{\rho} \quad (4)$$

is equivalent to the unconditional minimization of the *information functional* [40], defined as

$$I[\hat{\rho}] = -S + \lambda_0 (\text{Tr} \hat{\rho} - 1) + \beta (\text{Tr} \hat{\rho} \hat{H} - E) + \beta \sum_i \nu_i (\text{Tr} \hat{\rho} \hat{C}_i - C_i) , \quad (5)$$

in which the standard conditions (2) and (3) are included explicitly. The quantities λ_0 , β , and $\beta \nu_i$ are the appropriate Lagrange multipliers, with $\beta \equiv 1/T$ being inverse temperature. Minimizing the information functional (5) with respect to the statistical operator $\hat{\rho}$ gives

$$\hat{\rho} = \frac{1}{Z} e^{-\beta H} , \quad (6)$$

where $Z \equiv \exp(1 + \lambda_0)$ is the partition function and the *grand Hamiltonian*

$$H \equiv \hat{H} + \sum_i \nu_i \hat{C}_i \quad (7)$$

is introduced. The representative statistical ensemble, under constraints (1), (2), and (3), is then the pair $\{\mathcal{F}, \hat{\rho}\}$ of a space \mathcal{F} of microstates and the statistical operator (6), with the grand Hamiltonian (7). When one of the condition operators \hat{C}_i is the number-of-particle operator \hat{N} and the related Lagrange multiplier $\nu_i = -\mu$, one gets a particular form of the grand Hamiltonian $H = \hat{H} - \mu \hat{N}$. However, any other necessary constraints can be included, resulting in the general expression (7) for the grand Hamiltonian.

The condition operators \hat{C}_i are to be self-adjoint, $\hat{C}_i^+ = \hat{C}_i$, so that the grand Hamiltonian (7) be also self-adjoint. In many cases, the condition operators are taken as integrals of motion, such that $[\hat{C}_i, \hat{H}] = 0$. But this is not compulsory. For instance, the number-of-particle operator \hat{N} does not commute with the Hamiltonian energy operator \hat{H} , when the global gauge symmetry is broken.

The representative ensemble $\{\mathcal{F}, \hat{\rho}\}$, with the statistical operator (6) and the grand Hamiltonian (7), define all thermodynamics of an equilibrium, or stationary, system. The construction of this ensemble has been more or less straightforward, following the ideas of Gibbs [34], ter Haar [35,36], and Janes [37,38], as is reviewed in Refs. [5,40]. But the definition of representative ensembles for arbitrary nonequilibrium systems is not evident. Below, we give the generalization of the notion of representative ensembles for nonequilibrium statistical systems.

To describe a nonequilibrium system, one needs, in addition to the space of microstates \mathcal{F} and the initial value of the statistical operator $\hat{\rho} = \hat{\rho}(0)$, to define the temporal evolution of the system. This evolution can be described by the time-dependent statistical operators $\hat{\rho}(t)$, satisfying the Liouville equation, or by the time dependence of physical operators, satisfying the Heisenberg equation. Equivalently, the time evolution can be associated with the

evolution operator, satisfying the Schrödinger equation. Keeping in mind any of these ways, we may denote the prescribed temporal evolution by the symbol $\partial/\partial t$. Then a *nonequilibrium statistical ensemble* is a triplet $\{\mathcal{F}, \hat{\rho}, \partial/\partial t\}$. Clearly, when the time evolution is absent, or trivial, this definition reduces to that for the equilibrium case.

To be more specific, we may remember that each system is characterized by some dynamical variables, such as field operators. Let us keep in mind a set of field operators $\psi(x, t)$, whose particular representation is not important at this stage. For example, the variable x can represent real-space coordinates or momenta. It may also include other continuous or discrete variables, such as the spin indices or component labels. All physical operators, such as the Hamiltonian energy operator $\hat{H}[\psi]$, are functionals of the field operators.

The most general way for describing the system dynamics, as is known [41], is the extremization of the action functional. Implementing this for our case, we need the Lagrangian

$$\hat{L}[\psi] \equiv \hat{E}[\psi] - \hat{H}[\psi] , \quad (8)$$

in which the notation

$$\hat{E}[\psi] \equiv \int \psi^\dagger(x, t) i \frac{\partial}{\partial t} \psi(x, t) dx \quad (9)$$

for the temporal energy operator is used.

To make the ensemble representative, we have to take account of all additional conditions uniquely characterizing the system. This implies that, similarly to Eq. (1), we have to take care of the *statistical conditions*

$$C_i = \langle \hat{C}_i[\psi] \rangle , \quad (10)$$

where $\hat{C}_i[\psi]$ are the appropriate condition operators and

$$\langle \hat{C}_i[\psi] \rangle \equiv \text{Tr} \hat{\rho}(0) \hat{C}_i[\psi(x, t)] = \text{Tr} \hat{\rho}(t) \hat{C}_i[\psi(x, 0)] .$$

The principle of action extremization, under the given statistical conditions (10), is equivalent to the unconditional extremization of the effective action

$$A[\psi] = \int \left\{ \hat{L}[\psi] - \nu_i \hat{C}_i[\psi] \right\} dt \quad (11)$$

with the Lagrange multipliers ν_i guaranteeing the validity of conditions (10). Combining Eqs. (8) and (11), we can rewrite the effective action (11) as

$$A[\psi] = \int \left\{ \hat{E}[\psi] - H[\psi] \right\} dt , \quad (12)$$

with the *grand Hamiltonian*

$$H[\psi] \equiv \hat{H}[\psi] + \sum_i \nu_i \hat{C}_i[\psi] , \quad (13)$$

having the same form as in Eq. (7). The extremization of the action functional with respect to field operators means the variational equation

$$\frac{\delta A[\psi]}{\delta \psi^\dagger(x, t)} = 0 \quad (14)$$

plus its Hermitian conjugate. Equation (14), in view of action (12), is identical to the equation

$$i \frac{\partial}{\partial t} \psi(x, t) = \frac{\delta H[\psi]}{\delta \psi^\dagger(x, t)} . \quad (15)$$

The evolution equation (15) is what one needs for a complete definition of the nonequilibrium representative ensemble. It is important to stress that the system dynamics is governed by the same grand Hamiltonian as its thermodynamics.

We may also note that in the Heisenberg representation, as is well known (see, e.g., Refs. [40,41]), the variational equation (15) is the same as the Heisenberg equation

$$i \frac{\partial}{\partial t} \psi(x, t) = [\psi(x, t), H[\psi]] .$$

The time evolution of the field operators is given by the form

$$\psi(x, t) = \hat{U}^+(t) \psi(x, 0) \hat{U}(t) ,$$

expressed through the evolution operator $\hat{U}(t)$ satisfying the Schrödinger equation

$$i \frac{d}{dt} \hat{U}(t) = H[\psi(x, 0)] \hat{U}(t) .$$

Respectively, the time dependence of the statistical operator $\hat{\rho}(t)$ stems from the Liouville equation, yielding

$$\hat{\rho}(t) = \hat{U}(t) \hat{\rho}(0) \hat{U}^+(t) .$$

In any case, it is the grand Hamiltonian (13), which governs the temporal evolution of a nonequilibrium system.

3 Broken Gauge Symmetry

Now, let us specify the general notion of representative statistical ensembles, formulated above, for Bose systems, in which there exists the critical temperature T_c below which the global $U(1)$ gauge symmetry becomes broken. For concreteness, we keep in mind a one-component system of spinless particles, characterized by the field operators satisfying the Bose commutation relations.

Above the critical temperature T_c , the system is described by field operators $\psi = \psi(\mathbf{r}, t)$ and the conjugate ψ^\dagger , being functions of spatial, \mathbf{r} , and temporal, t , variables. These operators generate the Fock space $\mathcal{F}(\psi)$ on which all physical operators are defined. The related mathematical details can be found in the books [40–42]. The Hamiltonian energy operator $\hat{H}[\psi]$ is a gauge-invariant functional of the field operators. The number-of-particle operator $\hat{N}[\psi]$ is normalized to the total number of particles $N = \langle \hat{N}[\psi] \rangle$. Therefore the grand Hamiltonian is

$$H[\psi] = \hat{H}[\psi] - \mu \hat{N}[\psi] \quad (T > T_c) .$$

This grand Hamiltonian, entering the statistical operator (6), characterizes the representative statistical ensemble for the normal Bose system, above the critical temperature, where the global gauge symmetry is preserved.

Below the critical temperature T_c , the global gauge symmetry becomes broken. The symmetry breaking is realized by the Bogolubov shift

$$\psi(\mathbf{r}, t) \longrightarrow \hat{\psi}(\mathbf{r}, t) \equiv \eta(\mathbf{r}, t) + \psi_1(\mathbf{r}, t) , \quad (16)$$

where $\eta(\mathbf{r}, t)$ is the condensate wave function, while $\psi_1(\mathbf{r}, t)$ is the field operator of uncondensed particles. The field operators ψ_1 and ψ_1^\dagger generate the Fock space $\mathcal{F}(\psi_1)$, which all physical operators are to be defined on. In Eq. (16), the condensate wave function $\eta(\mathbf{r}, t)$, strictly speaking, is assumed to be factored with the unity operator $\hat{1}_{\mathcal{F}}$ in $\mathcal{F}(\psi_1)$. However here and in what follows, we shall use the common way of omitting the explicit appearance of the unity operator, in order not to make formulas too cumbersome. The condensate function $\eta(\mathbf{r}, t)$ can also be termed as the coherent field, since the related coherent state $|\eta\rangle$ is the vacuum state in the space $\mathcal{F}(\psi_1)$. This and other mathematical details can be found in Refs. [40,42,43].

Thus, instead of one field variable $\psi(\mathbf{r}, t)$ above T_c , for the Bose system below T_c , where the gauge symmetry is broken, there arise two field variables, the condensate function (coherent field) $\eta(\mathbf{r}, t)$ and the field operator $\psi_1(\mathbf{r}, t)$ of uncondensed particles. These two dynamical variables are, of course, assumed to be linearly independent, being orthogonal to each other,

$$\int \eta^*(\mathbf{r}, t) \psi_1(\mathbf{r}, t) d\mathbf{r} = 0 . \quad (17)$$

It is of principal importance to emphasize that the spaces $\mathcal{F}(\psi)$ for $T > T_c$ and $\mathcal{F}(\psi_1)$ for $T < T_c$ are mutually orthogonal [43,44]. The field operators ψ and ψ_1 are defined on different spaces, $\mathcal{F}(\psi)$ and $\mathcal{F}(\psi_1)$, respectively, realizing two different unitary nonequivalent operator representations, with the Bose commutation relations [43,44]. As soon as the gauge symmetry is broken, one has to deal with the space $\mathcal{F}(\psi_1)$. It would be principally incorrect to work, first, in the space $\mathcal{F}(\psi)$, accomplishing there some transformations, and then to pass to the space $\mathcal{F}(\psi_1)$ by breaking the symmetry with the Bogolubov shift (16). As is shown in Ref. [6], such a procedure leads to wrong results. From the mathematical point of view, it is absolutely obvious that any manipulations must be accomplished in one given space, where all operators are defined.

Now, in the space $\mathcal{F}(\psi_1)$, we have two normalization conditions for two linearly independent field variables, $\eta(\mathbf{r}, t)$ and $\psi_1(\mathbf{r}, t)$. The condensate function is normalized to the number of condensed particles

$$N_0 = \int |\eta(\mathbf{r}, t)|^2 d\mathbf{r} , \quad (18)$$

which is assumed to be macroscopic, such that the condensate fraction N_0/N be nonzero in the thermodynamic limit. This normalization can be rewritten in the standard form of the statistical conditions (10) by using the operator

$$\hat{N}_0 \equiv N_0 \hat{1}_{\mathcal{F}} , \quad (19)$$

where $\hat{1}_{\mathcal{F}}$ is the unity operator in $\mathcal{F}(\psi_1)$. Then Eq. (18) transforms to the statistical condition

$$N_0 = \langle \hat{N}_0 \rangle , \quad (20)$$

in which, as in what follows, the averaging is over the space $\mathcal{F}(\psi_1)$. The second normalization is, clearly, for the number of uncondensed particles

$$N_1 = \langle \hat{N}_1 \rangle , \quad (21)$$

with the corresponding operator

$$\hat{N}_1 \equiv \int \psi_1^\dagger(\mathbf{r}, t) \psi_1(\mathbf{r}, t) d\mathbf{r} . \quad (22)$$

The total number of particles

$$N = \langle \hat{N} \rangle = N_0 + N_1 \quad (23)$$

is the average of the operator

$$\hat{N} \equiv \int \hat{\psi}^\dagger(\mathbf{r}, t) \hat{\psi}(\mathbf{r}, t) d\mathbf{r} = \hat{N}_0 + \hat{N}_1 . \quad (24)$$

Normalization (23) follows from Eqs. (20) and (21). Therefore, among three normalization conditions, (20), (21), and (23), only two can be treated as independent. Generally, any combination of the pairs, for N_0 and N_1 , or for N_0 and N , or for N_1 and N , could be chosen. For the sake of symmetry, we prefer to choose the normalization conditions (20) and (21).

When the gauge symmetry is broken, the average $\langle \psi_1 \rangle$ may become nonzero. This, however, would mean that quantum numbers, as spin or momentum, are not conserved. In order to avoid this unpleasant situation, one has to impose an additional constraint

$$\langle \psi_1(\mathbf{r}, t) \rangle = 0 . \quad (25)$$

The latter can be reduced to the standard form of the statistical conditions (10) by defining a self-adjoint operator

$$\hat{\Lambda}[\psi_1] \equiv \int \left[\lambda(\mathbf{r}, t) \psi_1^\dagger(\mathbf{r}, t) + \lambda^*(\mathbf{r}, t) \psi_1(\mathbf{r}, t) \right] d\mathbf{r} , \quad (26)$$

in which $\lambda(\mathbf{r}, t)$ is a complex function. Then constraint (25) can be rewritten as the *quantum-number conservation condition*

$$\langle \hat{\Lambda}[\psi_1] \rangle = 0 . \quad (27)$$

In this way, for the correct representation of a Bose system with broken gauge symmetry, we must work in the space $\mathcal{F}(\psi_1)$ and take into account three statistical conditions, (20), (21), and (27). The corresponding representative ensemble is constructed following the general procedure, formulated in Sec. 2.

For an equilibrium system, according to Eq. (5), we have the information functional

$$\begin{aligned} I[\hat{\rho}] = & \text{Tr} \hat{\rho} \ln \hat{\rho} + \lambda_0 (\text{Tr} \hat{\rho} - 1) + \beta \left(\text{Tr} \hat{\rho} \hat{H}[\eta, \psi_1] - E \right) \\ & - \beta \mu_0 \left(\text{Tr} \hat{\rho} \hat{N}_0 - N_0 \right) - \beta \mu_1 \left(\text{Tr} \hat{\rho} \hat{N}_1 - N_1 \right) - \beta \text{Tr} \hat{\rho} \hat{\Lambda}[\psi_1] . \end{aligned} \quad (28)$$

Minimizing the latter yields the statistical operator

$$\hat{\rho} = \frac{1}{Z} \exp \{ -\beta H[\eta, \psi_1] \} , \quad (29)$$

with the partition function

$$Z \equiv \text{Tr} \exp \{ -\beta H[\eta, \psi_1] \} ,$$

and the grand Hamiltonian

$$H[\eta, \psi_1] \equiv \hat{H}[\eta, \psi_1] - \mu_0 \hat{N}_0 - \mu_1 \hat{N}_1 - \hat{\Lambda}[\psi_1] , \quad (30)$$

in agreement with Eq. (7).

For the general case of a nonequilibrium system, we have the Lagrangian

$$\hat{L}[\eta, \psi_1] = \hat{E}[\eta, \psi_1] - \hat{H}[\eta, \psi_1] ,$$

in which

$$\hat{E}[\eta, \psi_1] = \int \left\{ \eta^*(\mathbf{r}, t) i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) + \psi_1^\dagger(\mathbf{r}, t) i \frac{\partial}{\partial t} \psi_1(\mathbf{r}, t) \right\} d\mathbf{r} .$$

Then, similarly to Eq. (12), the effective action is

$$A[\eta, \psi_1] = \int \left\{ \hat{E}[\eta, \psi_1] - H[\eta, \psi_1] \right\} dt , \quad (31)$$

with the same grand Hamiltonian (30). Since we have now two linearly independent field variables, the extremization of action (31) gives two variational equations, for the condensate function,

$$\frac{\delta A[\eta, \psi_1]}{\delta \eta^*(\mathbf{r}, t)} = 0 , \quad (32)$$

and for the field operators of uncondensed particles,

$$\frac{\delta A[\eta, \psi_1]}{\delta \psi_1^\dagger(\mathbf{r}, t)} = 0 . \quad (33)$$

Equations (32) and (33), in view of the effective action (31), are equivalent to the evolution equations

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \frac{\delta H[\eta, \psi_1]}{\delta \eta^*(\mathbf{r}, t)} \quad (34)$$

and, respectively,

$$i \frac{\partial}{\partial t} \psi_1(\mathbf{r}, t) = \frac{\delta H[\eta, \psi_1]}{\delta \psi_1^\dagger(\mathbf{r}, t)} . \quad (35)$$

And, as usual, these equations are to be complimented by their Hermitian conjugate.

Thus, the representative statistical ensemble $\{\mathcal{F}(\psi_1), \hat{\rho}, \partial/\partial t\}$ for a Bose system with broken global gauge symmetry is defined in complete agreement with the general theory of Sec. 2. The dynamics and thermodynamics of such a system are governed by the grand Hamiltonian (30). It is only by accurately taking into account all imposed constraints that it is possible to correctly define the representative ensemble and to develop a self-consistent theory, avoiding any internal defects and paradoxes. The imposed statistical conditions (20), (21), and (27) lead to the grand Hamiltonian (30), with the Lagrange multipliers μ_0 , μ_1 , and $\lambda(\mathbf{r}, t)$. The form of this Hamiltonian is more general than that of the trivial expression $\hat{H} - \mu \hat{N}$. For a system with broken gauge symmetry, the number of the Lagrange multipliers in the form $\hat{H} - \mu \hat{N}$ is smaller than the number of imposed constraints. As a result, the problem becomes mathematically overdefined, which leads to the inconsistencies described in Sec. 1.

4 Self-Consistent Thermodynamic Relations

For an equilibrium system, the condensate function does not depend on time, $\eta(\mathbf{r}, t) = \eta(\mathbf{r})$. The grand thermodynamic potential

$$\Omega = -T \ln \text{Tr} \exp(-\beta H[\eta, \psi_1]) \quad (36)$$

is defined through the grand Hamiltonian (30). As is evident by this definition,

$$\frac{\partial \Omega}{\partial \mu_0} = -N_0, \quad \frac{\partial \Omega}{\partial \mu_1} = -N_1.$$

Varying potential (36) with respect to $\eta(\mathbf{r})$ gives the equation

$$\frac{\delta \Omega}{\delta \eta^*(\mathbf{r})} = \left\langle \frac{\delta H[\eta, \psi_1]}{\delta \eta^*(\mathbf{r})} \right\rangle = 0 \quad (37)$$

for the condensate function, in agreement with Eq. (34), when in equilibrium $\partial \eta(\mathbf{r})/\partial t = 0$. In order that the system with Bose-Einstein condensate be stable, the thermodynamic potential (36) is to be minimal with respect to the number of condensed particles N_0 , so that

$$\frac{\delta \Omega}{\delta N_0} = \left\langle \frac{\partial H[\eta, \psi_1]}{\partial N_0} \right\rangle = 0, \quad (38)$$

which is the Bogolubov-Ginibre stability condition. Under normalization (18), the dependence on N_0 comes through the condensate function $\eta(\mathbf{r})$, because of which

$$\frac{\partial \Omega}{\partial N_0} = \int \left[\frac{\delta \Omega}{\delta \eta(\mathbf{r})} \frac{\partial \eta(\mathbf{r})}{\partial N_0} + \frac{\delta \Omega}{\delta \eta^*(\mathbf{r})} \frac{\partial \eta^*(\mathbf{r})}{\partial N_0} \right] d\mathbf{r}.$$

Therefore Eq. (38) is a direct consequence of Eq. (37). Of course, for a uniform system, Eqs. (37) and (38) identically coincide.

The average densities of condensed, uncondensed, and all particles are

$$\rho_0 \equiv \frac{N_0}{V}, \quad \rho_1 \equiv \frac{N_1}{V}, \quad \rho \equiv \frac{N}{V}, \quad (39)$$

respectively. The related fractions of condensed and uncondensed particles are

$$n_0 \equiv \frac{N_0}{N} \equiv \frac{\rho_0}{\rho}, \quad n_1 \equiv \frac{N_1}{N} \equiv \frac{\rho_1}{\rho}. \quad (40)$$

From these definitions, one has

$$\rho = \rho_0 + \rho_1, \quad n_0 + n_1 = 1. \quad (41)$$

What one can usually fix in experiment is temperature T and the total density ρ .

The system free energy writes as

$$F = \Omega + \mu_0 N_0 + \mu_1 N_1. \quad (42)$$

Recall that $N_0 = N_0(T, \rho)$ is such that to guarantee the system thermodynamic stability. From the equations of motion, together with the relation $N = N_0 + N_1$, one finds $N_1 =$

$N_1(T, \rho)$. As is mentioned above, in experiment, only the total number of particles can be fixed, except temperature and volume. Hence, the free energy can be written as

$$F = \Omega + \mu N , \quad (43)$$

which can be considered as the definition of the system chemical potential μ . Comparing Eqs. (42) and (43) gives

$$\mu = \mu_0 n_0 + \mu_1 n_1 . \quad (44)$$

Then one can define the free energy $F = F(T, V, N)$ as a function of temperature, volume, and the total number of particles, with the differential

$$dF = -S dT - P dV + \mu dN , \quad (45)$$

in which S is entropy and P is pressure. From here, all measurable thermodynamic quantities are calculated in the standard way. For example, the system chemical potential is

$$\mu = \left(\frac{\partial F}{\partial N} \right)_{TV} . \quad (46)$$

As is evident, Eqs. (44) and (46) are identical by the above definitions.

At zero temperature, the free energy $F = E - TS$ reduces to the internal energy

$$E \equiv \langle \hat{H}[\eta, \psi_1] \rangle = \langle H[\eta, \psi_1] \rangle + \mu N . \quad (47)$$

Therefore the chemical potential (46) becomes

$$\mu = \left(\frac{\partial E}{\partial N} \right)_V \quad (T = 0) .$$

The grand potential (36) is a function $\Omega = \Omega(T, V, \mu)$ of temperature, volume, and chemical potential, with the differential

$$d\Omega = -S dT - P dV - N d\mu . \quad (48)$$

It is easy to check that the thermodynamic and Gibbs entropies coincide, so that

$$S = - \frac{\partial \Omega}{\partial T} = -\text{Tr} \hat{\rho} \ln \hat{\rho} . \quad (49)$$

This immediately follows from the direct differentiation of the grand potential (36) and the form of the statistical operator (29).

It is also possible to prove (see the proof in the Appendix A), that the standard relation

$$\frac{\partial N}{\partial \mu} = \beta \Delta^2(\hat{N}) \quad (50)$$

holds, in which $\Delta^2(\hat{N})$ is the dispersion of the number-of-particle operator $\hat{N} = \hat{N}_0 + \hat{N}_1$. The dispersion of a self-adjoint operator \hat{A} is

$$\Delta^2(\hat{A}) \equiv \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2 .$$

In this way, all thermodynamics quantities and relations are defined self-consistently.

5 Operator Equations of Motion

The equations of motion for the field variables $\eta(\mathbf{r}, t)$ and $\psi_1(\mathbf{r}, t)$ are given by Eqs. (34) and (35). To specify them, let us take the Hamiltonian energy operator in the standard form

$$\begin{aligned} \hat{H}[\eta, \psi_1] = & \int \hat{\psi}^\dagger(\mathbf{r}) \left(-\frac{\nabla^2}{2m} + U \right) \hat{\psi}(\mathbf{r}) d\mathbf{r} \\ & + \frac{1}{2} \int \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') \Phi(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) d\mathbf{r} d\mathbf{r}', \end{aligned} \quad (51)$$

in which $\hat{\psi}(\mathbf{r}) = \hat{\psi}(\mathbf{r}, t)$ is the shifted field operator defined in Eq. (16). In order to avoid cumbersome notations, we omit the explicit dependence on time of the variables $\eta(\mathbf{r}) = \eta(\mathbf{r}, t)$ and $\psi_1(\mathbf{r}) = \psi_1(\mathbf{r}, t)$, though this dependence is assumed. In what follows, such an abbreviated notation will be often used, where it does not lead to confusion. The external potential $U = U(\mathbf{r}, t)$ can, in general, depend on time. The interaction potential $\Phi(\mathbf{r})$ is arbitrary, provided it is symmetric, such that $\Phi(\mathbf{r}) = \Phi(-\mathbf{r})$, and enjoys the Fourier transformation.

The grand Hamiltonian (30) can be written as a sum of five terms,

$$H[\eta, \psi_1] = \sum_{n=0}^4 H^{(n)}, \quad (52)$$

whose order is labelled by the number of operators ψ_1 in their products. The zero-order term contains no ψ_1 , being

$$\begin{aligned} H^{(0)} = & \int \eta^*(\mathbf{r}) \left(-\frac{\nabla^2}{2m} + U - \mu_0 \right) \eta(\mathbf{r}) d\mathbf{r} \\ & + \frac{1}{2} \int \Phi(\mathbf{r} - \mathbf{r}') |\eta(\mathbf{r}')|^2 |\eta(\mathbf{r})|^2 d\mathbf{r} d\mathbf{r}'. \end{aligned} \quad (53)$$

To satisfy the quantum-number conservation condition (27), the Hamiltonian must not contain the terms linear in ψ_1 . This prescribes to take the Lagrange multipliers in Eq. (26) as

$$\lambda(\mathbf{r}, t) = \left[-\frac{\nabla^2}{2m} + U + \int \Phi(\mathbf{r} - \mathbf{r}') |\eta(\mathbf{r}', t)|^2 d\mathbf{r}' \right] \eta(\mathbf{r}, t), \quad (54)$$

so that $H^{(1)} = 0$. The necessity of removing the terms linear in ψ_1 or ψ_1^\dagger , by means of condition (54), in order to satisfy constraint (25), can be easily proved for quadratic Hamiltonians, involving linear terms, by employing the method of canonical transformations [42,45]. In the general case of arbitrary Hamiltonians, the proof of Eq. (54), yielding the cancellation of linear terms, is presented in the Appendix B.

The second-order term is

$$\begin{aligned} H^{(2)} = & \int \psi_1^\dagger(\mathbf{r}) \left(-\frac{\nabla^2}{2m} + U - \mu_1 \right) \psi_1(\mathbf{r}) d\mathbf{r} \\ & + \int \Phi(\mathbf{r} - \mathbf{r}') \left[|\eta(\mathbf{r})|^2 \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') + \eta^*(\mathbf{r}) \eta(\mathbf{r}') \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}) \right. \\ & \left. + \frac{1}{2} \eta^*(\mathbf{r}) \eta^*(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) + \frac{1}{2} \eta(\mathbf{r}) \eta(\mathbf{r}') \psi_1^\dagger(\mathbf{r}') \psi_1^\dagger(\mathbf{r}) \right] d\mathbf{r} d\mathbf{r}'. \end{aligned} \quad (55)$$

Respectively, we have the third-order term

$$H^{(3)} = \int \Phi(\mathbf{r} - \mathbf{r}') \left[\eta^*(\mathbf{r}) \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) + \psi_1^\dagger(\mathbf{r}) \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \eta(\mathbf{r}) \right] d\mathbf{r} d\mathbf{r}' \quad (56)$$

and the fourth-order term

$$H^{(4)} = \frac{1}{2} \int \psi_1^\dagger(\mathbf{r}) \psi_1^\dagger(\mathbf{r}') \Phi(\mathbf{r} - \mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) d\mathbf{r} d\mathbf{r}' . \quad (57)$$

From Eq. (34), we obtain

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \left(-\frac{\nabla^2}{2m} + U - \mu_0 \right) \eta(\mathbf{r}, t) + \int \Phi(\mathbf{r} - \mathbf{r}') \left[|\eta(\mathbf{r}')|^2 \eta(\mathbf{r}) + \hat{X}(\mathbf{r}, \mathbf{r}') \right] d\mathbf{r}' , \quad (58)$$

where the last term in the integrand is the correlation operator

$$\begin{aligned} \hat{X}(\mathbf{r}, \mathbf{r}') &\equiv \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \eta(\mathbf{r}) \\ &+ \psi_1^\dagger(\mathbf{r}') \eta(\mathbf{r}') \psi_1(\mathbf{r}) + \eta^*(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) + \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) . \end{aligned} \quad (59)$$

And Eq. (35) yields

$$\begin{aligned} i \frac{\partial}{\partial t} \psi_1(\mathbf{r}, t) &= \left(-\frac{\nabla^2}{2m} + U - \mu_1 \right) \psi_1(\mathbf{r}, t) \\ &+ \int \Phi(\mathbf{r} - \mathbf{r}') \left[|\eta(\mathbf{r}')|^2 \psi_1(\mathbf{r}) + \eta^*(\mathbf{r}') \eta(\mathbf{r}) \psi_1(\mathbf{r}') + \eta(\mathbf{r}') \eta(\mathbf{r}) \psi_1^\dagger(\mathbf{r}') + \hat{X}(\mathbf{r}, \mathbf{r}') \right] d\mathbf{r}' . \end{aligned} \quad (60)$$

Again, for brevity, the time dependence is not explicitly shown in the integrals of Eqs. (59) and (60). Also, recall that in the operator equation (58), the condensate function is assumed to be factored with $\hat{1}_{\mathcal{F}}$, the unity operator in $\mathcal{F}(\psi_1)$.

6 Local Conservation Laws

The equations of motion (58) and (60) are derived from the variational principle of action extremization. Therefore they guarantee the validity of all local conservation laws on the operator level. As an illustration, let us consider the time variation of the local densities.

The local condensate density is

$$\rho_0(\mathbf{r}, t) \equiv |\eta(\mathbf{r}, t)|^2 , \quad (61)$$

and the local condensate current is

$$\mathbf{j}_0(\mathbf{r}, t) \equiv -\frac{i}{2m} [\eta^*(\mathbf{r}, t) \nabla \eta(\mathbf{r}, t) - \eta(\mathbf{r}, t) \nabla \eta^*(\mathbf{r}, t)] . \quad (62)$$

Respectively, we define the operator density of uncondensed particles

$$\hat{\rho}_1(\mathbf{r}, t) \equiv \psi_1^\dagger(\mathbf{r}, t) \psi_1(\mathbf{r}, t) \quad (63)$$

and the related current operator

$$\mathbf{j}_1(\mathbf{r}, t) \equiv -\frac{i}{2m} \left\{ \psi_1^\dagger(\mathbf{r}, t) \nabla \psi_1(\mathbf{r}, t) - [\nabla \psi_1^\dagger(\mathbf{r}, t)] \psi_1(\mathbf{r}, t) \right\} . \quad (64)$$

Differentiating the condensate density (61), we find

$$\frac{\partial}{\partial t} \rho_0(\mathbf{r}, t) + \nabla \cdot \mathbf{j}_0(\mathbf{r}, t) = -\hat{\Gamma}(\mathbf{r}, t) , \quad (65)$$

where the source operator is

$$\hat{\Gamma}(\mathbf{r}, t) \equiv \int \Phi(\mathbf{r} - \mathbf{r}') \left[\hat{R}(\mathbf{r}, \mathbf{r}') + \hat{R}^+(\mathbf{r}, \mathbf{r}') \right] d\mathbf{r}' , \quad (66)$$

in which

$$\hat{R}(\mathbf{r}, \mathbf{r}') \equiv i\eta^*(\mathbf{r}) \left[\psi_1^\dagger(\mathbf{r}')\eta(\mathbf{r}') + \eta^*(\mathbf{r}')\psi_1(\mathbf{r}') + \psi_1^\dagger(\mathbf{r}')\psi_1(\mathbf{r}') \right] \psi_1(\mathbf{r}) .$$

And the time variation of density (63) yields

$$\frac{\partial}{\partial t} \hat{\rho}_1(\mathbf{r}, t) + \nabla \cdot \hat{\mathbf{j}}_1(\mathbf{r}, t) = \hat{\Gamma}(\mathbf{r}, t) . \quad (67)$$

For the total operator density

$$\hat{\rho}(\mathbf{r}, t) = \rho_0(\mathbf{r}, t) + \hat{\rho}_1(\mathbf{r}, t) \quad (68)$$

and the total operator of current

$$\hat{\mathbf{j}}(\mathbf{r}, t) = \mathbf{j}_0(\mathbf{r}, t) + \hat{\mathbf{j}}_1(\mathbf{r}, t) , \quad (69)$$

we obtain the *continuity equation*

$$\frac{\partial}{\partial t} \rho(\mathbf{r}, t) + \nabla \cdot \hat{\mathbf{j}}(\mathbf{r}, t) = 0 . \quad (70)$$

In the same way, one can derive any other local conservation laws, following the standard procedure [40,45] and employing the equations of motion (58) and (60).

7 Condensate Wave Function

The equation for the condensate wave function $\eta(\mathbf{r}, t)$ follows from averaging Eq. (58) over $\mathcal{F}(\psi_1)$. To this end, we need to introduce several notations. The normal density matrix is

$$\rho_1(\mathbf{r}, \mathbf{r}') \equiv \langle \psi_1^\dagger(\mathbf{r}')\psi_1(\mathbf{r}) \rangle . \quad (71)$$

Under the broken gauge symmetry, there appears the so-called anomalous density matrix

$$\sigma_1(\mathbf{r}, \mathbf{r}') \equiv \langle \psi_1(\mathbf{r}')\psi_1(\mathbf{r}) \rangle . \quad (72)$$

The density of condensed particles is $\rho_0(\mathbf{r})$, defined in Eq. (61), and the density of uncondensed particles is

$$\rho_1(\mathbf{r}) \equiv \rho_1(\mathbf{r}, \mathbf{r}) = \langle \psi_1^\dagger(\mathbf{r})\psi_1(\mathbf{r}) \rangle . \quad (73)$$

We shall also need the anomalous average

$$\sigma_1(\mathbf{r}) \equiv \sigma_1(\mathbf{r}, \mathbf{r}) = \langle \psi_1(\mathbf{r})\psi_1(\mathbf{r}) \rangle . \quad (74)$$

The absolute value $|\sigma_1(\mathbf{r})|$ has the meaning of the density of pair-correlated particles [43]. The total density

$$\rho(\mathbf{r}) = \rho_0(\mathbf{r}) + \rho_1(\mathbf{r}) \quad (75)$$

is the average of the operator density (68). According to the normalization conditions (20) and (21), the partial densities are normalized to the number of corresponding particles,

$$N_0 = \int \rho_0(\mathbf{r}) d\mathbf{r} , \quad N_1 = \int \rho_1(\mathbf{r}) d\mathbf{r} . \quad (76)$$

One more notation is the triple correlator

$$\xi(\mathbf{r}, \mathbf{r}') \equiv \langle \psi_1^\dagger(\mathbf{r}') \psi_1(\mathbf{r}') \psi_1(\mathbf{r}) \rangle . \quad (77)$$

Using these definitions, the average of the correlation operator (59) becomes

$$\langle \hat{X}(\mathbf{r}, \mathbf{r}') \rangle = \rho_1(\mathbf{r}') \eta(\mathbf{r}) + \rho_1(\mathbf{r}, \mathbf{r}') \eta(\mathbf{r}') + \sigma_1(\mathbf{r}, \mathbf{r}') \eta^*(\mathbf{r}') + \xi(\mathbf{r}, \mathbf{r}') .$$

Finally, averaging Eq. (58) yields the evolution equation for the condensate wave function

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \left(-\frac{\nabla^2}{2m} + U - \mu_0 \right) \eta(\mathbf{r}, t) + \int \Phi(\mathbf{r} - \mathbf{r}') [\rho(\mathbf{r}') \eta(\mathbf{r}) + \rho_1(\mathbf{r}, \mathbf{r}') \eta(\mathbf{r}') + \sigma_1(\mathbf{r}, \mathbf{r}') \eta^*(\mathbf{r}') + \xi(\mathbf{r}, \mathbf{r}')] d\mathbf{r}' . \quad (78)$$

This is the general equation for an arbitrary Bose-condensed system. This equation can also be represented in a shorter, though not explicit, form

$$i \frac{\partial}{\partial t} \eta(\mathbf{r}, t) = \left(-\frac{\nabla^2}{2m} + U - \mu_0 \right) \eta(\mathbf{r}, t) + \int \Phi(\mathbf{r} - \mathbf{r}') \langle \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) \rangle d\mathbf{r}' ,$$

in which one has to substitute the shifted operator $\hat{\psi} = \eta + \psi_1$.

We may notice that Eq. (78) is invariant under the transformation

$$\eta(\mathbf{r}, t) \longrightarrow \eta(\mathbf{r}, t) e^{i\alpha t} , \quad \psi_1(\mathbf{r}, t) \longrightarrow \psi_1(\mathbf{r}, t) e^{i\alpha t} , \quad \mu_0 \longrightarrow \mu_0 + \alpha . \quad (79)$$

This means that there exists a freedom in choosing the phase factor $\exp(i\alpha t)$ of the condensate function. But the phase factor becomes fixed by defining the Lagrange multiplier μ_0 . The arbitrariness in the condensate phase implies that the stationary solutions for $\eta(\mathbf{r}, t)$ would be proportional to an undefined factor $e^{i\alpha t}$. By fixing the multiplier μ_0 , we require that in equilibrium the condensate function would not be dependent on time, that is,

$$\frac{\partial}{\partial t} \eta(\mathbf{r}) = 0 \quad (\text{equilibrium}) . \quad (80)$$

In equilibrium, Eq. (78), according to condition (80), reduces to the eigenvalue problem

$$\mu_0 \eta(\mathbf{r}) = \left[-\frac{\nabla^2}{2m} + U(\mathbf{r}) \right] \eta(\mathbf{r}) + \int \Phi(\mathbf{r} - \mathbf{r}') [\rho(\mathbf{r}') \eta(\mathbf{r}) + \rho_1(\mathbf{r}, \mathbf{r}') \eta(\mathbf{r}') + \sigma_1(\mathbf{r}, \mathbf{r}') \eta^*(\mathbf{r}') + \xi(\mathbf{r}, \mathbf{r}')] d\mathbf{r}' , \quad (81)$$

defining, together with the normalization condition (76), the eigenfunction $\eta(\mathbf{r})$ and the eigenvalue μ_0 . Let us emphasize that without the normalization condition (76) the condensate function cannot be uniquely defined from Eq. (81). For example, if the system is uniform, with no external potential $U \rightarrow 0$, when $\eta(\mathbf{r}) = \eta$, $\rho(\mathbf{r}) = \rho$, and $\eta = \sqrt{\rho_0}$, then Eq. (81) gives

$$\mu_0 = \rho\Phi_0 + \int \Phi(\mathbf{r}) \left[\rho_1(\mathbf{r}, 0) + \sigma_1(\mathbf{r}, 0) + \frac{\xi(\mathbf{r}, 0)}{\sqrt{\rho_0}} \right] d\mathbf{r} , \quad (82)$$

where $\Phi_0 \equiv \int \Phi(\mathbf{r}) d\mathbf{r}$, or in the compact form

$$\mu_0 = \frac{1}{\sqrt{\rho_0}} \int \Phi(\mathbf{r}) < \hat{\psi}^\dagger(0) \hat{\psi}(0) \hat{\psi}(\mathbf{r}) > d\mathbf{r} .$$

Expression (82) is valid for an arbitrary uniform equilibrium system with an interaction potential $\Phi(\mathbf{r})$. No approximations have been used in obtaining Eq. (82).

In recent days, the physics of dilute Bose gases is intensively explored (see the book [46] and review articles [31,47–49]). The interaction potential for these gases is taken in the contact form

$$\Phi(\mathbf{r}) = \Phi_0 \delta(\mathbf{r}) , \quad \Phi_0 \equiv 4\pi \frac{a_s}{m} , \quad (83)$$

where a_s is the scattering length. With this interaction potential, the eigenvalue problem (81) for a nonuniform system becomes

$$\begin{aligned} \mu_0 \eta(\mathbf{r}) = & \left[-\frac{\nabla^2}{2m} + U(\mathbf{r}) \right] \eta(\mathbf{r}) \\ & + \Phi_0 \{ [\rho(\mathbf{r}) + \rho_1(\mathbf{r})] \eta + \sigma_1(\mathbf{r}) \eta^*(\mathbf{r}) + \xi(\mathbf{r}, \mathbf{r}) \} . \end{aligned} \quad (84)$$

For a uniform system, μ_0 is given by Eq. (82), which, in the case of the contact potential (83), yields

$$\mu_0 = \left(\rho + \rho_1 + \sigma_1 + \frac{\xi}{\sqrt{\rho_0}} \right) \Phi_0 , \quad (85)$$

where $\sigma_1 \equiv \sigma_1(\mathbf{r}, \mathbf{r})$ and $\xi \equiv \xi(\mathbf{r}, \mathbf{r})$.

When one assumes that the Bose gas is dilute, being characterized by the contact potential (83), the temperature is zero, and the interaction is so weak that the condensate depletion can be neglected, so that all particles are condensed, then $N_0 = N$, $N_1 = 0$, and $\rho_1 = \sigma_1 = \xi = 0$. In this approximation, because of relation (44), the multiplier $\mu_0 = \mu$ coincides with the system chemical potential. The eigenvalue problem (84) reduces then to the Gross-Pitaevskii equation

$$\left[-\frac{\nabla^2}{2m} + U(\mathbf{r}) + \Phi_0 |\eta(\mathbf{r})|^2 \right] \eta(\mathbf{r}) = \mu \eta(\mathbf{r}) .$$

But when the condensate depletion is not negligible, then μ_0 , according to Eq. (44), is not the same as μ .

8 Uniform Bose system

Let us illustrate in more detail the application of the representative ensemble with the grand Hamiltonian (52), to an equilibrium uniform system. Then the field operators of uncondensed particles can be expanded in plane waves,

$$\psi_1(\mathbf{r}) = \sum_{k \neq 0} a_k \varphi_k(\mathbf{r}) , \quad (86)$$

where $\varphi_k(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} / \sqrt{V}$. The condensate function reduces to the constant $\eta = \sqrt{\rho_0}$, while the condensate multiplier μ_0 is given by Eq. (82).

In the momentum representation, the momentum distribution of particles

$$n_k \equiv \langle a_k^\dagger a_k \rangle \quad (87)$$

is usually termed the normal average, as compared to the anomalous average

$$\sigma_k \equiv \langle a_k a_{-k} \rangle . \quad (88)$$

The normal and anomalous density matrices (71) and (72) take the form of the expansions

$$\rho_1(\mathbf{r}, \mathbf{r}') = \sum_{k \neq 0} n_k \varphi_k(\mathbf{r}) \varphi_k^*(\mathbf{r}') , \quad \sigma_1(\mathbf{r}, \mathbf{r}') = \sum_{k \neq 0} \sigma_k \varphi_k(\mathbf{r}) \varphi_k^*(\mathbf{r}') , \quad (89)$$

in which the properties

$$\langle a_k^\dagger a_p \rangle = \delta_{kp} n_k , \quad \langle a_k a_p \rangle = \delta_{-kp} \sigma_k$$

are taken into account. The diagonal elements of the matrices in Eq. (89) give the densities

$$\rho_1 = \rho_1(\mathbf{r}, \mathbf{r}) = \frac{1}{V} \sum_{k \neq 0} n_k , \quad \sigma_1 = \sigma_1(\mathbf{r}, \mathbf{r}) = \frac{1}{V} \sum_{k \neq 0} \sigma_k . \quad (90)$$

The interaction potential is assumed to allow the Fourier transformation

$$\Phi(\mathbf{r}) = \frac{1}{V} \sum_k \Phi_k e^{i\mathbf{k} \cdot \mathbf{r}} \quad \Phi_k = \int \Phi(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}} d\mathbf{r} . \quad (91)$$

Then we find the following terms of the grand Hamiltonian (52). The zero-order term (53) becomes

$$H^{(0)} = \left(\frac{1}{2} \rho_0 \Phi_0 - \mu_0 \right) N_0 . \quad (92)$$

The first-order term $H^{(1)} = 0$ is automatically zero. The second-order term (55) is

$$H^{(2)} = \sum_{k \neq 0} \left[\frac{k^2}{2m} + \rho_0 (\Phi_0 + \Phi_k) - \mu_1 \right] a_k^\dagger a_k + \frac{1}{2} \sum_{k \neq 0} \rho_0 \Phi_k (a_k^\dagger a_{-k}^\dagger + a_{-k} a_k) . \quad (93)$$

For the third-order term (56), we have

$$H^{(3)} = \sqrt{\frac{\rho_0}{V}} \sum'_{kp} \Phi_p (a_k^\dagger a_{k+p} a_{-p} + a_{-p}^\dagger a_{k+p}^\dagger a_k) , \quad (94)$$

where the prime on the summation symbol implies that $\mathbf{k} \neq 0$, $\mathbf{p} \neq 0$, $\mathbf{k} + \mathbf{p} \neq 0$. The fourth-order term (57) is

$$H^{(4)} = \frac{1}{2V} \sum_q \sum_{kp}' \Phi_q a_k^\dagger a_p^\dagger a_{p+q} a_{k-q} , \quad (95)$$

where the prime shows that $\mathbf{k} \neq 0$, $\mathbf{p} \neq 0$, $\mathbf{p} + \mathbf{q} \neq 0$, $\mathbf{k} - \mathbf{q} \neq 0$.

To be more specific, it is necessary to resort to some approximation. The natural mean-field approximation for a system with broken gauge symmetry is the HFB approximation. The latter is usually blamed to display an unphysical gap in the spectrum, because of which it is qualified as gapful (see detailed discussion in Refs. [7,31,32]). However, as is explained in the Introduction, this defect comes into play only owing to the usage of a nonrepresentative statistical ensemble. But for the representative ensemble, with the grand Hamiltonian (52), there appear no such problems. Below, we show this for the case of arbitrary temperature and interaction potential $\Phi(\mathbf{r})$.

We apply, in the standard way [40,45], the HFB approximation to the third- and fourth-order products of the operators a_k . Then the third-order term (94) becomes identically zero, because of the condition $\langle a_k \rangle = 0$,

$$H^{(3)} = 0 . \quad (96)$$

And for the fourth-order term (95), we get

$$\begin{aligned} H^{(4)} = & \sum_{k \neq 0} \rho_1 \Phi_0 \left(a_k^\dagger a_k - \frac{1}{2} n_k \right) \\ & + \frac{1}{V} \sum_{k,p \neq 0} \Phi_k \left[n_{k+p} a_p^\dagger a_p + \frac{1}{2} \left(\sigma_{k+p} a_p^\dagger a_{-p}^\dagger + \sigma_{k+p}^* a_{-p} a_p \right) - \frac{1}{2} (n_{k+p} n_p + \sigma_{k+p} \sigma_p) \right] . \end{aligned} \quad (97)$$

It is convenient to introduce the notations

$$\omega_k \equiv \frac{k^2}{2m} + \rho \Phi_0 + \rho_0 \Phi_k + \frac{1}{V} \sum_{p \neq 0} n_p \Phi_{k+p} - \mu_1 \quad (98)$$

and

$$\Delta_k \equiv \rho_0 \Phi_k + \frac{1}{V} \sum_{p \neq 0} \sigma_p \Phi_{k+p} . \quad (99)$$

Since the interaction potential $\Phi(\mathbf{r}) = \Phi(-\mathbf{r})$ is symmetric and real, we have the properties $\sigma_k = \sigma_k^* = \sigma_{-k}$ and $\Delta_k = \Delta_k^* = \Delta_{-k}$.

Summing up all terms in the grand Hamiltonian (52), we obtain in the HFB approximation

$$H_{HFB} = E_{HFB} + \sum_{k \neq 0} \omega_k a_k^\dagger a_k + \frac{1}{2} \sum_{k \neq 0} \Delta_k \left(a_k^\dagger a_{-k}^\dagger + a_{-k} a_k \right) , \quad (100)$$

where the nonoperator term is

$$E_{HFB} = H^{(0)} - \frac{1}{2} \rho_1^2 \Phi_0 V - \frac{1}{2V} \sum_{k,p \neq 0} \Phi_{k+p} (n_k n_p + \sigma_k \sigma_p) . \quad (101)$$

The quadratic form (100) can be diagonalized by the Bogolubov canonical transformation [3,4,45]

$$a_k = u_k b_k + v_{-k}^* b_{-k}^\dagger .$$

As a result, the grand Hamiltonian (100) is transformed to the Bogolubov representation

$$H_B = E_B + \sum_{k \neq 0} \varepsilon_k b_k^\dagger b_k , \quad (102)$$

in which

$$E_B = E_{HFB} + \frac{1}{2} \sum_{k \neq 0} (\varepsilon_k - \omega_k) . \quad (103)$$

For the operators b_k , one has the properties

$$\langle b_k \rangle = \langle b_k b_p \rangle = 0 , \quad \langle b_k^\dagger b_p \rangle = \delta_{kp} \pi_k , \quad (104)$$

with the momentum distribution of quasiparticles

$$\pi_k \equiv \langle b_k^\dagger b_k \rangle = (e^{\beta \varepsilon_k} - 1)^{-1} = \frac{1}{2} \left[\coth \left(\frac{\varepsilon_k}{2T} \right) - 1 \right] . \quad (105)$$

The coefficient functions u_k and v_k , and the spectrum ε_k are defined by the Bogolubov - de Gennes equations

$$(\omega_k - \varepsilon_k) u_k + \Delta_k v_k = 0 , \quad \Delta_k u_k + (\omega_k + \varepsilon_k) v_k = 0 ,$$

with the normalization condition $u_k^2 - v_k^2 = 1$. This gives

$$u_k^2 = \frac{\omega_k + \varepsilon_k}{2\varepsilon_k} , \quad v_k^2 = \frac{\omega_k - \varepsilon_k}{2\varepsilon_k} .$$

And the Bogolubov spectrum is

$$\varepsilon_k = \sqrt{\omega_k^2 - \Delta_k^2} . \quad (106)$$

The existence of the Bose-Einstein condensate, as is known, requires that the spectrum (106) be gapless, such that

$$\lim_{k \rightarrow 0} \varepsilon_k = 0 , \quad (107)$$

with the stability condition $\varepsilon_k \geq 0$. Then Eq. (106) yields

$$\mu_1 = \rho \Phi_0 + \frac{1}{V} \sum_{p \neq 0} (n_p - \sigma_p) \Phi_p . \quad (108)$$

As will be shown in Sec. 10, this value is in exact agreement with the Hugenholtz-Pines relation. This should be compared with the condensate potential (82), which in the HFB approximation, when $\xi(\mathbf{r}, \mathbf{r}') = 0$, becomes

$$\mu_0 = \rho \Phi_0 + \frac{1}{V} \sum_{p \neq 0} (n_p + \sigma_p) \Phi_p . \quad (109)$$

In the particular case of the contact potential (83), we get

$$\mu_1 = (\rho + \rho_1 - \sigma_1) \Phi_0 \quad (110)$$

and, respectively,

$$\mu_0 = (\rho + \rho_1 + \sigma_1)\Phi_0 . \quad (111)$$

In any case, generally, $\mu_0 \neq \mu_1$. The multipliers μ_0 and μ_1 become equal only in the limit of the asymptotically small condensate depletion, which corresponds to the Bogolubov approximation [1,2], when both ρ_1 and σ_1 in Eqs. (108) to (111) are neglected. Then, clearly, $\mu_0 = \mu_1 = \rho_0\Phi_0$, and in view of relation (44), $\mu_0 = \mu_1 = \mu$. However, as soon as the condensate depletion is not negligible, $\mu_0 \neq \mu_1$.

With the multiplier (108), Eq. (98) can be represented as

$$\omega_k = \frac{k^2}{2m} + \rho_0\Phi_k + \frac{1}{V} \sum_{p \neq 0} (n_p\Phi_{k+p} - n_p\Phi_p + \sigma_p\Phi_p) . \quad (112)$$

For the long-wave limit of Δ_k , we introduce the notation

$$\Delta \equiv \lim_{k \rightarrow 0} \Delta_k \equiv mc^2 . \quad (113)$$

From Eq. (99) it follows

$$\Delta = \rho_0\Phi_0 + \frac{1}{V} \sum_{p \neq 0} \sigma_p\Phi_p . \quad (114)$$

Then the long-wave limit of spectrum (106) is explicitly of the phonon type, $\varepsilon \simeq ck$, as $k \rightarrow 0$. According to the notation (113), the sound velocity is

$$c = \sqrt{\frac{\Delta}{m}} . \quad (115)$$

Strictly speaking, the sound velocity is defined as $c = \sqrt{\Delta/m^*}$, with an effective mass to be given in Sec. 10. For short-range interactions, $m^* \cong m$. Using Eqs. (113) and (114), we may rewrite Eq. (112) in the form

$$\omega_k = \frac{k^2}{2m} + mc^2 + \rho_0(\Phi_k - \Phi_0) + \int n_p(\Phi_{k+p} - \Phi_p) \frac{d\mathbf{k}}{(2\pi)^3} . \quad (116)$$

For the particle momentum distribution (87), we find

$$n_k = \frac{\omega_k}{2\varepsilon_k} \coth\left(\frac{\varepsilon_k}{2T}\right) - \frac{1}{2} , \quad (117)$$

while for the anomalous average (88), we obtain

$$\sigma_k = -\frac{\Delta_k}{2\varepsilon_k} \coth\left(\frac{\varepsilon_k}{2T}\right) . \quad (118)$$

Analyzing the behaviour of n_k and σ_k as functions of momentum k , we find [15,32] that $|\sigma_k| \simeq n_k$ for $k \rightarrow 0$, while $|\sigma_k| \gg n_k$ for large k . Therefore in no sense the anomalous average σ_k can be neglected, as compared to the normal average n_k .

The derived equations simplify for the contact potential (83). Then $\Phi_k = \Phi_0$, $\Delta_k = \Delta$,

$$\Delta = (\rho_0 + \sigma_1)\Phi_0 ,$$

and spectrum (106) takes the classical Bogolubov form

$$\varepsilon_k = \sqrt{(ck)^2 + \left(\frac{k^2}{2m}\right)^2} . \quad (119)$$

The grand potential (36) in the HFB approximation is

$$\Omega = E_B + TV \int \ln \left(1 - e^{-\beta \varepsilon_k}\right) \frac{d\mathbf{k}}{(2\pi)^3} . \quad (120)$$

From this and other equations, obtained above, all thermodynamic characteristics can be calculated.

9 Condensate and Superfluid Fractions

We shall concentrate our attention on the most interesting characteristics of the Bose-condensed system, on the condensate and superfluid fractions. The condensate fraction

$$n_0 = 1 - \frac{\rho_1}{\rho} \quad (121)$$

can be found by calculating the density ρ_1 of uncondensed particles, given by the integral

$$\rho_1 = \int n_k \frac{d\mathbf{k}}{(2\pi)^3} . \quad (122)$$

To define the superfluid fraction, one considers the reaction of the system to the boost with a velocity \mathbf{v} . In the laboratory frame, the field operators of a moving system are represented by means of the Galilean transformation

$$\hat{\psi}_v(\mathbf{r}, t) = \hat{\psi}(\mathbf{r} - \mathbf{v}t, t) \exp \left\{ i \left(m\mathbf{v} \cdot \mathbf{r} - \frac{mv^2}{2} t \right) \right\} . \quad (123)$$

The Hamiltonian $H_v = H[\hat{\psi}_v]$, in terms of the new field operators (123), is expressed through the Hamiltonian $H = H[\hat{\psi}]$, in terms of the old operators $\hat{\psi}$, as

$$H_v = H + \int \hat{\psi}^\dagger(\mathbf{r}) \left(-i\mathbf{v} \cdot \nabla + \frac{mv^2}{2} \right) \hat{\psi}(\mathbf{r}) d\mathbf{r} . \quad (124)$$

The total system momentum operator becomes

$$\hat{\mathbf{P}}_v = \hat{\mathbf{P}} + Nm\mathbf{v} , \quad (125)$$

where

$$\hat{\mathbf{P}} = \int \hat{\psi}^\dagger(\mathbf{r})(-i\nabla)\hat{\psi}(\mathbf{r}) d\mathbf{r} \quad (126)$$

is the old momentum operator. The average total momentum of the moving system is

$$\langle \hat{\mathbf{P}}_v \rangle_v \equiv \text{Tr} \hat{\rho}_v \hat{\mathbf{P}}_v , \quad (127)$$

with the statistical operator

$$\hat{\rho}_v \equiv \frac{e^{-\beta H_v}}{\text{Tr} e^{-\beta H_v}} . \quad (128)$$

The superfluid fraction is defined as

$$n_s \equiv \frac{1}{3mN} \lim_{v \rightarrow 0} \frac{\partial}{\partial \mathbf{v}} \cdot \langle \hat{\mathbf{P}}_v \rangle_v . \quad (129)$$

It is possible to show (see, e.g., the detailed derivation in Refs. [47,49]) that the superfluid fraction (129) for an arbitrary system can be represented in the form

$$n_s = 1 - \frac{2Q}{3T} , \quad (130)$$

in which

$$Q \equiv \frac{\Delta^2(\hat{\mathbf{P}})}{2mN} \quad (131)$$

is the *dispersed heat*, with the momentum dispersion

$$\Delta^2(\hat{\mathbf{P}}) \equiv \langle \hat{\mathbf{P}}^2 \rangle - \langle \hat{\mathbf{P}} \rangle^2 ,$$

where the averages are with respect to the grand Hamiltonian $H[\hat{\psi}]$.

Formula (130) for the superfluid fraction is valid for any system, equilibrium or nonequilibrium, uniform or not. For a system in equilibrium, the total momentum is zero, $\langle \hat{\mathbf{P}} \rangle = 0$, so that the dispersed heat (131) is

$$Q = \frac{\langle \hat{\mathbf{P}}^2 \rangle}{2mN} . \quad (132)$$

For a uniform system,

$$\langle \hat{\mathbf{P}}^2 \rangle = \sum_{kp} (\mathbf{k} \cdot \mathbf{p}) \langle \hat{n}_k \hat{n}_p \rangle , \quad (133)$$

where $\hat{n}_k \equiv a_k^\dagger a_k$. In the HFB approximation,

$$\langle \hat{n}_k \hat{n}_p \rangle = n_k n_p + \delta_{kp} n_k (1 + n_k) + \delta_{-kp} \sigma_k^2 . \quad (134)$$

Then the dispersed heat (132) becomes

$$Q = \frac{1}{\rho} \int \frac{k^2}{2m} (n_k + n_k^2 - \sigma_k^2) \frac{d\mathbf{k}}{(2\pi)^3} . \quad (135)$$

Substituting here expressions (117) and (118), and using the equality $\cosh x - 1 = 2 \sinh^2(x/2)$, so that

$$n_k + n_k^2 - \sigma_k^2 = \frac{1}{4 \sinh^2(\beta \varepsilon_k / 2)} ,$$

we get from Eq. (135)

$$Q = \frac{1}{(4\pi)^2 m \rho} \int_0^\infty \frac{k^4 dk}{\sinh^2(\beta \varepsilon_k / 2)} . \quad (136)$$

Note again the importance of the anomalous average σ_k . If one would omit the latter in the dispersed heat (135), one would get a senseless divergent quantity, while accurately taking account of σ_k results in the well-defined convergent integral (136).

To demonstrate explicitly the behaviour of the condensate and superfluid fractions, let us resort to the contact potential (83). Then Eq. (99) yields

$$\Delta_k = \Delta = mc^2, \quad (137)$$

and Eq. (116) gives

$$\omega_k = \frac{k^2}{2m} + mc^2. \quad (138)$$

Equation (115), defining the sound velocity, can be written as

$$mc^2 = (\rho_0 + \sigma_1)\Phi_0, \quad (139)$$

where

$$\sigma_1 = \int \sigma_k \frac{d\mathbf{k}}{(2\pi)^3}. \quad (140)$$

The density of uncondensed particles (122) can be represented in the form

$$\rho_1 = \frac{(mc)^3}{3\pi^2} \left\{ 1 + \frac{3}{2\sqrt{2}} \int_0^\infty (\sqrt{1+x^2} - 1)^{1/2} \left[\coth\left(\frac{mc^2}{2T} x\right) - 1 \right] dx \right\}, \quad (141)$$

which is a well-defined convergent integral.

The anomalous average (140) can be written as a sum of two parts

$$\sigma_1 = \sigma_0 - \int \frac{mc^2}{2\varepsilon_k} \left[\coth\left(\frac{\varepsilon_k}{2T}\right) - 1 \right] \frac{d\mathbf{k}}{(2\pi)^3}, \quad (142)$$

in which

$$\sigma_0 \equiv -\Delta \int \frac{1}{2\varepsilon_k} \frac{d\mathbf{k}}{(2\pi)^3}. \quad (143)$$

The second integral in Eq. (142) is convergent. But the integral in Eq. (143) ultravioletly diverges. However, this divergence is known to be unphysical, being simply caused by the usage of the contact interaction potential. This and other similar divergences could be removed by employing more realistic interaction potentials. For example, a common choice is a Gaussian type potential [50]. Another known way of removing such divergences is by using the analytic regularization in one of its variants, such as the subtraction scheme, zeta regularization, or dimensional regularization (see details in Ref. [31]). This kind of regularization is asymptotically exact for weak interactions and is universal in the sense that it applies to any short-range potential with a scattering length a_s [31]. Using the dimensional regularization in its region of validity, we obtain

$$\int \frac{1}{2\varepsilon_k} \frac{d\mathbf{k}}{(2\pi)^3} = -\frac{m}{\pi^2} \sqrt{m\rho_0\Phi_0}.$$

Then Eq. (143) results in

$$\sigma_0 = \frac{(mc)^2}{\pi^2} \sqrt{m\rho_0\Phi_0}. \quad (144)$$

The anomalous average (142) can be represented as

$$\sigma_1 = \sigma_0 - \frac{(mc)^3}{2\sqrt{2}\pi^2} \int_0^\infty \frac{(\sqrt{1+x^2}-1)^{1/2}}{\sqrt{1+x^2}} \left[\coth\left(\frac{mc^2}{2T}x\right) - 1 \right] dx. \quad (145)$$

And for the dispersed heat (136), we obtain

$$Q = \frac{(mc)^5}{\sqrt{2}(2\pi)^2 m\rho} \int_0^\infty \frac{(\sqrt{1+x^2}-1)^{3/2} x dx}{\sqrt{1+x^2} \sinh^2(mc^2 x/2T)}. \quad (146)$$

At low temperatures, such that

$$\frac{T}{mc^2} \ll 1,$$

equations (141), (145), and (146) yield

$$\begin{aligned} \rho_1 &\simeq \frac{(mc)^3}{3\pi^2} + \frac{(mc)^3}{12} \left(\frac{T}{mc^2}\right)^2, & \sigma_1 &\simeq \sigma_0 - \frac{(mc)^3}{12} \left(\frac{T}{mc^2}\right)^2, \\ Q &\simeq \frac{\pi^2(mc)^5}{15m\rho} \left(\frac{T}{mc^2}\right)^5. \end{aligned}$$

Therefore, the condensate fraction (121) behaves as

$$n_0 \simeq 1 - \frac{(mc)^3}{3\pi^2\rho} - \frac{(mc)^3}{12\rho} \left(\frac{T}{mc^2}\right)^2. \quad (147)$$

And the superfluid fraction (130) becomes

$$n_s \simeq 1 - \frac{2\pi^2(mc)^3}{45\rho} \left(\frac{T}{mc^2}\right)^4. \quad (148)$$

When the interaction is weak, or the condensate fraction n_0 tends to zero at the critical temperature T_c , as a results of which, $c \rightarrow 0$, so that

$$\frac{mc^2}{T_c} \ll 1,$$

then Eqs. (141), (145), and (146) lead to

$$\begin{aligned} \rho_1 &\simeq \rho \left(\frac{T}{T_c}\right)^{3/2} + \frac{(mc)^3}{3\pi^2}, & \sigma_1 &\simeq \sigma_0 - \frac{m^2 c T}{2\pi}, \\ Q &\simeq \frac{3}{2} T \left[\left(\frac{T}{T_c}\right)^{3/2} - \frac{\zeta(1/2)}{\zeta(3/2)} \left(\frac{T}{T_c}\right)^{1/2} \frac{mc^2}{T_c} \right], \end{aligned}$$

with the critical temperature

$$T_c = \frac{2\pi}{m} \left[\frac{\rho}{\zeta(3/2)} \right]^{2/3}$$

coinciding with that for the ideal Bose gas, as it should be in the case of the mean-field approximation with the contact potential (83). Here $\zeta(\cdot)$ is the Riemann zeta function. Then the condensate fraction tends to zero at T_c as

$$n_0 \simeq 1 - \left(\frac{T}{T_c}\right)^{3/2} - \frac{(mc)^3}{3\pi^2\rho}, \quad (149)$$

together with the superfluid fraction

$$n_s \simeq 1 - \left(\frac{T}{T_c}\right)^{3/2} + \frac{\zeta(1/2)}{\zeta(3/2)} \left(\frac{T}{T_c}\right)^{1/2} \frac{mc^2}{T_c}. \quad (150)$$

Both, n_0 and n_s , tend to zero from the left, demonstrating the second-order phase transition at T_c . The point why in the present case T_c has to be the same as the ideal Bose gas critical temperature is explained in the Appendix C.

10 Green Function Equations

In order to conclude the proof of the complete self-consistency of the developed approach, based on the introduced representative ensemble, we need to show that for an arbitrary Bose system there exist the Green-function equations of the usual form and that the Hugenholtz-Pines relation follows for any uniform system.

The first-order Green function is defined in the standard way [3,4,7,9] as the matrix $G(12) = [G_{\alpha\beta}(12)]$ with the elements

$$\begin{aligned} G_{11}(12) &= -i \langle \hat{T} \psi_1(1) \psi_1^\dagger(2) \rangle, & G_{12}(12) &= -i \langle \hat{T} \psi_1(1) \psi_1(2) \rangle, \\ G_{21}(12) &= -i \langle \hat{T} \psi_1^\dagger(1) \psi_1^\dagger(2) \rangle, & G_{22}(12) &= -i \langle \hat{T} \psi_1^\dagger(1) \psi_1(2) \rangle, \end{aligned} \quad (151)$$

in which the common abbreviation is employed, denoting the set $\{\mathbf{r}_j, t_j\}$ by a single number j , and \hat{T} is the chronological operator.

For what follows, we shall need the notation for the triple field operator

$$\begin{aligned} \Psi(123) &\equiv \psi_1(1) \psi_1(2) \psi_1^\dagger(3) + \eta(1) \psi_1(2) \psi_1^\dagger(3) + \psi_1(1) \eta(2) \psi_1^\dagger(3) \\ &+ \psi_1(1) \psi_1(2) \eta^*(3) + \eta(1) \eta(2) \psi_1^\dagger(3) + \eta(1) \psi_1(2) \eta^*(3) + \psi_1(1) \eta(2) \eta^*(3). \end{aligned} \quad (152)$$

One may notice that

$$\Psi(123) = \hat{\psi}(1) \hat{\psi}(2) \hat{\psi}^\dagger(3) - \eta(1) \eta(2) \eta^*(3),$$

where $\hat{\psi} = \eta + \psi_1$ is the shifted field operator. However, for practical application, we need the explicit form (152).

The second-order Green function is a matrix $B(1234) = [B_{\alpha\beta}(1234)]$ with the elements

$$\begin{aligned} B_{11}(1234) &= - \langle \hat{T} \Psi(123) \psi_1^\dagger(4) \rangle, & B_{12}(1234) &= - \langle \hat{T} \Psi(123) \psi_1(4) \rangle, \\ B_{21}(1234) &= - \langle \hat{T} \Psi^\dagger(123) \psi_1^\dagger(4) \rangle, & B_{22}(1234) &= - \langle \hat{T} \Psi^\dagger(123) \psi_1(4) \rangle. \end{aligned} \quad (153)$$

For the general form of a retarded interaction potential

$$\Phi(12) \equiv \Phi(\mathbf{r}_1 - \mathbf{r}_2)\delta(t_{12} + 0) , \quad (154)$$

in which $t_{12} = t_1 - t_2$, the self-energy is introduced through the equation

$$\int \Sigma(13)G(32) d(3) = i \int \Phi(13)B(1332) d(3) . \quad (155)$$

The equation for $G(12)$, by defining the inverse propagator

$$G^{-1}(12) \equiv \left(\hat{\tau} i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} - U(1) + \mu_1 \right) \delta(12) \hat{1} - \Sigma(12) , \quad (156)$$

in which

$$\hat{\tau} \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} , \quad \hat{1} \equiv \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} ,$$

can be represented in the form

$$\int G^{-1}(13)G(32) d(3) = \delta(12) \hat{1} . \quad (157)$$

To solve Eq. (157), one may invoke perturbation theory, starting with an available approximate Green function G_{app} , corresponding to an approximate Σ_{app} , such that

$$\int G_{app}^{-1}(13)G_{app}(32) d(3) = \delta(12) \hat{1} . \quad (158)$$

Then Eqs. (157) and (158) can be transformed to the Dyson representation

$$G(12) = G_{app}(12) + \int G_{app}(13) [\Sigma(34) - \Sigma_{app}(34)] G(42) d(34) , \quad (159)$$

which is convenient for using perturbation theory.

The above equations for the Green functions are valid for an arbitrary nonequilibrium and nonuniform Bose system. If the considered system is equilibrium and uniform, one passes to the Fourier transforms $G(\mathbf{k}, \omega)$ and $\Sigma(\mathbf{k}, \omega)$, employing the symmetry properties

$$G_{11}(\mathbf{k}, -\omega) = G_{22}(\mathbf{k}, \omega) , \quad G_{12}(\mathbf{k}, -\omega) = G_{21}(\mathbf{k}, \omega) = G_{12}(\mathbf{k}, \omega) ,$$

$$G_{\alpha\beta}(-\mathbf{k}, \omega) = G_{\alpha\beta}(\mathbf{k}, \omega) \quad (160)$$

and, respectively,

$$\Sigma_{11}(\mathbf{k}, -\omega) = \Sigma_{22}(\mathbf{k}, \omega) , \quad \Sigma_{12}(\mathbf{k}, -\omega) = \Sigma_{21}(\mathbf{k}, \omega) = \Sigma_{12}(\mathbf{k}, \omega) ,$$

$$\Sigma_{\alpha\beta}(-\mathbf{k}, \omega) = \Sigma_{\alpha\beta}(\mathbf{k}, \omega) . \quad (161)$$

A detailed discussion of these relations can be found in Ref. [4].

Let us introduce the notation

$$D(\mathbf{k}, \omega) \equiv \Sigma_{12}^2(\mathbf{k}, \omega) - G_{11}^{-1}(\mathbf{k}, \omega)G_{11}^{-1}(\mathbf{k}, -\omega) , \quad (162)$$

in which

$$G_{11}^{-1}(\mathbf{k}, \omega) = \omega - \frac{k^2}{2m} - \Sigma_{11}(\mathbf{k}, \omega) + \mu_1 .$$

Then the solution to Eq. (157) can be written as

$$G_{11}(\mathbf{k}, \omega) = \frac{\omega + k^2/2m + \Sigma_{11}(\mathbf{k}, \omega) - \mu_1}{D(\mathbf{k}, \omega)} , \quad G_{12}(\mathbf{k}, \omega) = - \frac{\Sigma_{12}(\mathbf{k}, \omega)}{D(\mathbf{k}, \omega)} , \quad (163)$$

with the denominator (162).

For the Green functions $G_{\alpha\beta}(\mathbf{k}, 0)$ at zero energy there is the Bogolubov theorem [4] rigorously proving the validity of the inequalities

$$|G_{11}(\mathbf{k}, 0)| \geq \frac{mn_0}{2k^2} , \quad (164)$$

$$|G_{11}(\mathbf{k}, 0) - G_{12}(\mathbf{k}, 0)| \geq \frac{mn_0}{k^2} . \quad (165)$$

From Eq. (163), we have

$$G_{11}(\mathbf{k}, 0) = \frac{k^2/2m + \Sigma_{11}(\mathbf{k}, 0) - \mu_1}{D(\mathbf{k}, 0)} , \quad G_{12}(\mathbf{k}, 0) = - \frac{\Sigma_{12}(\mathbf{k}, 0)}{D(\mathbf{k}, 0)} ,$$

where

$$D(\mathbf{k}, 0) = \Sigma_{12}^2(\mathbf{k}, 0) - \left[\frac{k^2}{2m} + \Sigma_{11}(\mathbf{k}, 0) - \mu_1 \right]^2 .$$

Consequently,

$$G_{11}(\mathbf{k}, 0) - G_{12}(\mathbf{k}, 0) = \left[\mu_1 - \frac{k^2}{2m} + \Sigma_{12}(\mathbf{k}, 0) - \Sigma_{11}(\mathbf{k}, 0) \right]^{-1} .$$

Using this in Eq. (165), we get

$$\left| \mu_1 - \frac{k^2}{2m} + \Sigma_{12}(\mathbf{k}, 0) - \Sigma_{11}(\mathbf{k}, 0) \right| \leq \frac{k^2}{mn_0} .$$

Setting in the latter equation $\mathbf{k} \rightarrow 0$, we come to the Hugenholtz-Pines relation

$$\mu_1 = \Sigma_{11}(0, 0) - \Sigma_{12}(0, 0) . \quad (166)$$

Note that in the HFB approximation we have

$$\Sigma_{11}(0, 0) = (\rho + \rho_0)\Phi_0 + \frac{1}{V} \sum_{p \neq 0} n_p \Phi_p , \quad \Sigma_{12}(0, 0) = \rho_0 \Phi_0 + \frac{1}{V} \sum_{p \neq 0} \sigma_p \Phi_p .$$

Therefore Eq. (166) gives exactly the form of μ_1 in Eq. (108).

Relation (166) guarantees that the system spectrum is gapless and of the phonon character. The spectrum ε_k is given by the zeros of the Green functions (163), that is, by the equation

$$D(\mathbf{k}, \varepsilon_k) = 0 , \quad (167)$$

with Eq. (162). Equation (167) can be rewritten as

$$\varepsilon_k = \frac{1}{2} [\Sigma_{11}(\mathbf{k}, \varepsilon_k) - \Sigma_{22}(\mathbf{k}, \varepsilon_k)] + \sqrt{\omega_k^2 - \Sigma_{12}^2(\mathbf{k}, \varepsilon_k)} , \quad (168)$$

where the notation

$$\omega_k \equiv \frac{k^2}{2m} + \frac{1}{2} [\Sigma_{11}(\mathbf{k}, \varepsilon_k) + \Sigma_{22}(\mathbf{k}, \varepsilon_k)] - \mu_1$$

is used. From Eq. (168), it follows that $\varepsilon_k \rightarrow 0$, as $k \rightarrow 0$. Moreover, when the system is isotropic, its self-energy $\Sigma_{\alpha\beta}(\mathbf{k}, \varepsilon_k)$ depends only on the scalar k^2 . This implies the asymptotic, as $k \rightarrow 0$, expansion

$$\Sigma_{\alpha\beta}(\mathbf{k}, \varepsilon_k) \simeq \Sigma_{\alpha\beta}(0, 0) + \Sigma'_{\alpha\beta} k^2 ,$$

in which

$$\Sigma'_{\alpha\beta} \equiv \lim_{k \rightarrow 0} \frac{\partial}{\partial k^2} \Sigma_{\alpha\beta}(\mathbf{k}, \varepsilon_k) .$$

Using this expansion in spectrum (168) gives

$$\varepsilon_k \simeq ck , \quad c \equiv \sqrt{\frac{1}{m^*} \Sigma_{12}(0, 0)} , \quad (169)$$

which is the phonon spectrum, with the sound velocity c , where the effective mass is

$$m^* \equiv \frac{m}{1 + m(\Sigma'_{11} + \Sigma'_{22} - 2\Sigma'_{12})} . \quad (170)$$

It is useful to compare the Lagrange multipliers μ_0 and μ_1 given by their general expressions (82) and (166), which are valid for an arbitrary equilibrium uniform Bose system. These expressions are exact, with no approximations being involved. As is seen, anomalous averages enter μ_0 with the sign plus, while the anomalous self-energy enters μ_1 with the sign minus. This is why, in general, μ_0 cannot coincide with μ_1 . The HFB forms (108) and (109), or (110) and (111), are particular illustrations. It is easy to check that μ_0 coincides with μ_1 solely in the Bogolubov limit of asymptotically weak interactions, when $\Sigma_{11}(0, 0) \rightarrow (\rho + \rho_0)\Phi_0$, $\Sigma_{12}(0, 0) \rightarrow \rho_0\Phi_0$, and $\mu_0 \rightarrow \mu_1 \rightarrow \mu = \rho\Phi_0$. But in any higher-order approximation, $\mu_0 \neq \mu_1$. The assumption that μ_0 would be the same as μ_1 would make the theory not self-consistent and would return us back to the Hohenberg-Martin dilemma of conserving versus gapless theories.

11 Discussion

The main message of this paper is the necessity of employing representative ensembles for correctly describing statistical systems. A representative ensemble takes into account all imposed constraints and additional conditions that allow for a unique description of the considered system. It is only using a representative ensemble makes the theory self-consistent.

In the Bose system with broken global gauge symmetry, realized by the Bogolubov shift, there are two particle components, corresponding to condensed and uncondensed particles, with two related normalization conditions for N_0 and N_1 . This requires to introduce two

Lagrange multipliers, μ_0 and μ_1 , which makes the theory completely self-consistent in any approximation.

It is worth recalling that the introduction of several Lagrange multipliers is rather common for spin systems. There, the order parameter is the average spin, which, generally, is a three-component vector. The role of the effective chemical potential for spin systems is played, as is well known, by an external magnetic field, which is also a three-component vector. Hence, the number of effective chemical potentials for spin systems is equal to the number of components in the order parameter. Only then one is able to unambiguously define the average spin.

The suggested approach, introducing two Lagrange multipliers, does not contradict our physical understanding that the standard experiments fix, as independent variables, temperature, volume, and the total number of particles. To emphasize this once again, let us turn to the definition of the grand thermodynamic potential (36), from which it follows that it is a function $\Omega = \Omega(T, V, \mu_0, \mu_1)$, so that the free energy (42) is a function $F = F(T, V, N_0, N_1)$. The Lagrange multiplier μ_0 is defined from the stability condition, yielding $\mu_0 = \mu_0(T, V, N_0, N_1)$, according to Eqs. (81), (82), (84), (85), (109), and (111). The Lagrange multiplier μ_1 satisfies the Hugenholtz-Pines theorem, which gives $\mu_1 = \mu_1(T, V, N_0, N_1)$, in agreement with Eqs. (108), (110), and (166). The number of uncondensed particles is found from the direct calculation of the average (21) expressed through Eqs. (90), (122), (141), and like that, resulting in $N_1 = N_1(T, V, N_0, N)$. From here, since $N_0 = N - N_1$, it follows that $N_0 = N_0(T, V, N)$. Substituting it back to N_1 , one has $N_1 = N_1(T, V, N)$. Using these in the expressions for μ_0 and μ_1 , one gets $\mu_0 = \mu_0(T, V, N)$ and $\mu_1 = \mu_1(T, V, N)$. Then, from Eq. (44), it is evident that $\mu = \mu(T, V, N)$, or, inverting the latter relation, one has $N = N(T, V, \mu)$. Using this, the Lagrange multipliers μ_0 and μ_1 can be expressed as functions $\mu_0 = \mu_0(T, V, \mu)$ and $\mu_1 = \mu_1(T, V, \mu)$. Substituting this into the grand potential, we have $\Omega = \Omega(T, V, \mu)$, in line with Eq. (48). Respectively, the free energy becomes a function $F = F(T, V, N)$, in accordance with Eq. (45).

Thus, at the end, we work with the standard variables T, V , and N , which are usually fixed in experiments. All observable quantities are also expressed through these variables. So that the suggested approach is absolutely self-consistent, mathematically correct, and in agreement with physics.

Several words are to be said with regard to the phase-transition order of Bose-Einstein condensation. This transition is known to be of *second-order*, which is firmly based on several facts. First, there exists a general explanation, independent of the coupling strength, that this transition is of second-order. This can be found in the book by Patashinsky and Pokrovsky [51] (Chapter X, Section 2). As is also well known, the Hamiltonian of Bose systems is mathematically equivalent to what in quantum theory is termed the φ^4 model. The phase transition in this model has been studied in numerous works using the renormalization group approach, exhibiting the second-order transition [52]. The superfluid transition in liquid ^4He , which is believed to be accompanied by the Bose-Einstein condensation, is also a second-order transition. A large body of experimental data on measuring the continuous temperature dependence of the condensate fraction in superfluid helium has been summarized by Wirth and Hallock [53]. There exists abundant literature, both theoretical and experimental, on Bose-Einstein condensation in dilute trapped gases (see review works [46–49]) and references therein) and there are several computer simulations of this process [54–56]. Though Bose condensation in traps is smeared out by finite-size effects, the

subsequent increase of the number of particles unambiguously demonstrates that the condensation approaches the standard second-order phase transition. In addition, there have been many Monte Carlo calculations for uniform Bose systems with various interaction potentials. All these calculations, summarized in the review articles [57–59], clearly prove that Bose-Einstein condensation is a second-order transition. So, the second order of the Bose condensate transition has been established without any doubt. This especially concerns the general theoretical investigations [51,52] and rigorous Monte Carlo calculations [57,58].

The main idea of the present paper is the necessity of using representative ensembles for describing Bose-condensed systems. This implies that proper allowance must be made for all conditions which uniquely define the employed field variables. Here the consideration has been based on the classical Bogolubov approach [1–4] introducing two field variables, the condensate function η and the operator of uncondensed particles ψ_1 . By their definition, these variables are *independent* of each other. For a uniform system, the condensate corresponds to the zero-momentum state, while this state is excluded from the description of uncondensed particles. This is evident from definition (86) of ψ_1 , where $\mathbf{k} \neq 0$. The variables η and ψ_1 are also *orthogonal* to each other, in agreement with definition (17), which becomes obvious from Eq. (86), since

$$\frac{1}{\sqrt{V}} \int \psi_1(\mathbf{r}) d\mathbf{r} = \sum_{\mathbf{k} \neq 0} a_{\mathbf{k}} \delta_{\mathbf{k}0} = 0. \quad (171)$$

For so introduced independent orthogonal variables, it is necessary to define two normalization conditions and, respectively, two Lagrange multipliers controlling these normalization conditions. Only then there can be the assurance that the theory will be self-consistent in any calculations.

Of course, if the field variables are introduced in a different way, with some other conditions, this would require to define another ensemble, with the appropriate Lagrange multipliers, whose number could also be different. For example, Hugenholtz and Pines [9], as well as later Gavoret and Noziers [60], when deriving the Hugenholtz-Pines relation on the basis of thermodynamic properties, *did not use* the standard grand ensemble. Any attentive reader can immediately infer from the original works [9,60] that these authors have used a different ensemble. They treat a uniform equilibrium system, defining the number of condensed particles N_0 by minimizing the *internal energy* at zero temperature, which corresponds to the minimization of *free energy* at finite temperatures. After defining in that way $N_0 = N_0(\rho, T)$, the latter is explicitly substituted into the effective Hamiltonian $\hat{H} - \mu \hat{N}_1$, where \hat{N}_1 is the operator of *uncondensed* particles, but not of the total number of particles, as it would be in the standard grand Hamiltonian. Since $N_0 = N_0(\rho, T)$ has been explicitly substituted everywhere, one needs the sole Lagrange multiplier for the normalization of *uncondensed* particles. But mathematically this is absolutely equivalent to the introduction of an additional Lagrange multiplier μ_0 , as is done in the present paper, *before* substituting $N_0(\rho, T)$, which is defined later from the corresponding normalization condition. These ways, as is absolutely clear, are equivalent, but the latter method is more convenient for more general cases of nonuniform or nonequilibrium systems.

Another example is given by the approach advanced by Faddeev and Popov [61] and used later by Popov [12–14]. They define the field operator

$$\psi(\mathbf{r}) = \sqrt{\rho_0} + \psi_{FP}(\mathbf{r}), \quad (172)$$

in which the second part in the right-hand side,

$$\psi_{FP}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_k a_k e^{i\mathbf{k}\cdot\mathbf{r}} , \quad (173)$$

includes the term $a_0 \neq 0$ with $\mathbf{k} = 0$. This is contrary to the Bogolubov field operator of uncondensed particles (86), not containing this zero-momentum term. The Fourier transform c_k of the operator

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_k c_k e^{i\mathbf{k}\cdot\mathbf{r}}$$

is connected with the Fourier transform of ψ_{FP} by the equation

$$c_k = \delta_{0k} \sqrt{N_0} + a_k .$$

For the zero-momentum state, one has

$$c_0 = \sqrt{N_0} + a_0 .$$

Recall that in the Bogolubov case, one would have $c_0 = \sqrt{N_0}$. Thus, in the Faddeev-Popov approach, the condensate is not completely separated from uncondensed particles, but ψ_{FP} does contain the zero-momentum term a_0 . In other words, ψ_{FP} is not independent from ρ_0 . Moreover, the Faddeev-Popov representation (172) for ψ consists of two parts that are not orthogonal to each other,

$$\frac{1}{\sqrt{V}} \int \psi_{FP}(\mathbf{r}) d\mathbf{r} = a_0 \neq 0 ,$$

which is contrary to the Bogolubov case (171). Hence, ψ_{FP} is neither independent of $\sqrt{\rho_0}$ nor orthogonal to it, but both of them define the sole variable (172). As far as, in the Faddeev-Popov approach, $a_0 \neq 0$, the latter yields the interference terms in physical operators. For instance, here the number-of-particle operator becomes

$$\hat{N} \equiv \int \psi^\dagger(\mathbf{r})\psi(\mathbf{r}) d\mathbf{r} = N_0 + \sum_k a_k^\dagger a_k + \sqrt{N_0} (a_0^\dagger + a_0) . \quad (174)$$

This operator is normalized to the total number of particles, so that

$$N = \langle \hat{N} \rangle = N_0 + \sum_k \langle a_k^\dagger a_k \rangle , \quad (175)$$

which requires $\langle a_0 \rangle = 0$. Faddeev and Popov in their original paper [61] emphasized that their representation (172) is principally different from the Bogolubov shift (16) and discussed in detail the corresponding differences. Because in the Faddeev-Popov approach there is a single independent variable ψ , with the normalization condition (175), the appropriate representative ensemble here is the standard grand ensemble, with the grand Hamiltonian $\hat{H} - \mu\hat{N}$, though the number-of-particle operator (174) here is different from the Bogolubov form (24). More complicated forms of physical operators and the necessity to comply with relation (172) at each step of any calculational procedure make the usage of the Faddeev-Popov approach more complicated and quite inconvenient for mean-field type approximations. However, needless to say that a theory with one independent variable and,

respectively, with one Lagrange multiplier, is mathematically equivalent to the theory with two independent variables and two Lagrange multipliers. Which representation to choose is rather a matter of convenience.

It is even admissible to introduce no Lagrange multipliers and to deal with the canonical Gibbs ensemble. But the problem with the latter is that then one has to keep the total number of particles fixed not merely on the average but exactly at each step of any calculational procedure. This requires to work in a restricted Fock space, where the number-of-particle operator degenerates to the number $\hat{N} \equiv N$. To accomplish this, one may resort to the Girardeau-Arnouitt approach [24,25] introducing the so-called number-conserving field operators

$$\alpha_k = \hat{N}_0^{-1/2} a_0^\dagger a_k, \quad \alpha_k^\dagger = a_k^\dagger a_0 \hat{N}_0^{-1/2}.$$

This representation, however, is valid only when the number of condensed particles is large, $N_0 \gg 1$, so that it is not applicable in the vicinity of the condensation point, when $N_0 \rightarrow 0$. Also, such a canonical representation in approximate calculations yields, as is known [24], a gap in the spectrum. It was noticed by Girardeau [62] and showed by Takano [63] that to get a self-consistent theory in the canonical ensemble requires to use the whole Hamiltonian, without reducing it to approximate forms. But the theory with a whole Hamiltonian for interacting particles has no exact solution. So, the usage of the canonical ensemble is unpractical in analytic investigations, though it may be employed for numerical computations [64,65].

Concluding, the choice of an ensemble is, generally speaking, a matter of convenience. But in any case, the chosen ensemble must be representative, which necessitates to accurately take into account all conditions uniquely defining the considered system. The choice of an ensemble is intimately connected with the choice of the appropriate field variables, which should not be confused. Employing inappropriate variables, that is, using a nonrepresentative ensemble may result in the appearance of inconsistencies and paradoxes. For example, resorting to the canonical ensemble, one should use the Girardeau-Arnouitt representation with the number-conserving field operators [24,25] or the Carusotto-Castin-Dalibard representation based on stochastic fields [64,65]. If one prefers the standard grand ensemble, then the Faddeev-Popov representation is appropriate [61]. A nonstandard variant of the grand ensemble, due to Hugenholtz and Pines [9], can also be used. But when the classical Bogolubov representation [1–4] is chosen, where the field variables of condensed and uncondensed particles are separated from each other, being independent and orthogonal, then the approach developed in the present paper is the most convenient, being completely self-consistent.

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Appendix A

Here we prove relation (50). From definition (36) for the grand potential with Hamiltonian (30), it immediately follows that

$$N_0 = - \frac{\partial \Omega}{\partial \mu_0} , \quad N_1 = - \frac{\partial \Omega}{\partial \mu_1} .$$

On the other hand,

$$N = - \frac{\partial \Omega}{\partial \mu} = N_0 + N_1 .$$

Comparing the above equations, we get

$$\frac{\partial \Omega}{\partial \mu} = \frac{\partial \Omega}{\partial \mu_0} + \frac{\partial \Omega}{\partial \mu_1} .$$

Differentiating again the latter equation, we have

$$\frac{\partial^2 \Omega}{\partial \mu^2} = \frac{\partial^2 \Omega}{\partial \mu_0^2} + \frac{\partial^2 \Omega}{\partial \mu_1^2} + 2 \frac{\partial^2 \Omega}{\partial \mu_0 \partial \mu_1} .$$

By direct calculations, we find that

$$\frac{\partial^2 \Omega}{\partial \mu_0^2} = -\beta \Delta^2(\hat{N}_0) , \quad \frac{\partial^2 \Omega}{\partial \mu_1^2} = -\beta \Delta^2(\hat{N}_1) , \quad \frac{\partial^2 \Omega}{\partial \mu_0 \partial \mu_1} = -\beta \text{cov}(\hat{N}_0, \hat{N}_1) ,$$

where the covariance of two operators, \hat{A} and \hat{B} , is

$$\text{cov}(\hat{A}, \hat{B}) \equiv \frac{1}{2} \langle \hat{A}\hat{B} + \hat{B}\hat{A} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle .$$

Summarizing these equations, and using the property of the dispersion of a composite operator,

$$\Delta^2(\hat{A} + \hat{B}) = \Delta^2(\hat{A}) + \Delta^2(\hat{B}) + 2\text{cov}(\hat{A}, \hat{B}) ,$$

we obtain

$$\frac{\partial N}{\partial \mu} = - \frac{\partial^2 \Omega}{\partial \mu^2} = \beta \Delta^2(\hat{N}) ,$$

which proves relation (50).

Appendix B

The fact that the terms linear in ψ_1 or ψ_1^\dagger must be absent in the Hamiltonian, in order to satisfy constraint (25), can be proved in two ways.

We may, first, consider a quadratic Hamiltonian approximating the exact one. Linear terms in such a Hamiltonian can also be present. Quadratic Hamiltonians of this type can be diagonalized with the help of exact canonical transformations [45]. Rigorous mathematical properties of the corresponding transformations, called nonuniform, are expounded in the book by Berezin [42]. After the Hamiltonian is diagonalized, it is straightforward to calculate explicitly all averages, which show that the linear terms in the Hamiltonian induce nonzero $\langle \psi_1 \rangle$ and, vice versa, zero linear terms lead to $\langle \psi_1 \rangle = 0$. Then one should consider perturbation theory, starting with the diagonalized quadratic form, and check that zero linear terms yield $\langle \psi_1 \rangle = 0$ in all orders of the theory. This way is rather cumbersome, and below another method is presented.

Let us consider the general Hamiltonian (52). Its term, linear in ψ_1 and ψ_1^\dagger , is

$$H^{(1)} = \int \psi_1^\dagger(\mathbf{r}) \left(-\frac{\nabla^2}{2m} + U \right) \eta(\mathbf{r}) d\mathbf{r} + \int \psi_1(\mathbf{r}) \left(-\frac{\nabla^2}{2m} + U \right) \eta^*(\mathbf{r}) d\mathbf{r} \\ + \int \Phi(\mathbf{r} - \mathbf{r}') \left[\psi_1^\dagger(\mathbf{r}) |\eta(\mathbf{r}')|^2 \eta(\mathbf{r}) + \eta^*(\mathbf{r}) |\eta(\mathbf{r}')|^2 \psi_1(\mathbf{r}) \right] d\mathbf{r} d\mathbf{r}' .$$

The equation of motion (35) can be represented as

$$i \frac{\partial}{\partial t} \psi_1(\mathbf{r}, t) = \frac{\delta[H - H^{(1)}]}{\delta \psi_1^\dagger(\mathbf{r}, t)} + \frac{\delta H^{(1)}}{\delta \psi_1^\dagger(\mathbf{r}, t)} .$$

The first term here gives the right-hand side of Eq. (60). The second term results in the form

$$\frac{\delta H^{(1)}}{\delta \psi_1^\dagger(\mathbf{r}, t)} = C(\mathbf{r}, t) \hat{1}_{\mathcal{F}} ,$$

proportional to the unit operator $\hat{1}_{\mathcal{F}}$ in the Fock space $\mathcal{F}(\psi_1)$ generated by the field operators ψ_1^\dagger , with the nonoperator complex function

$$C(\mathbf{r}, t) \equiv \left[-\frac{\nabla^2}{2m} + U + \int \Phi(\mathbf{r} - \mathbf{r}') |\eta(\mathbf{r}', t)|^2 d\mathbf{r}' \right] \eta(\mathbf{r}, t) - \lambda(\mathbf{r}, t) .$$

The equation of motion, written above, is an operator equality defined on $\mathcal{F}(\psi_1)$. The operator equality assumes that it holds true at least in the weak sense implying the equality of all matrix elements for the states from the space the operators are defined on. In the present case, the latter means the space $\mathcal{F}(\psi_1)$. The vacuum state of this space is defined in the standard way as the vector $|0\rangle$, for which $\psi_1(\mathbf{r}, t)|0\rangle = 0$. Considering for the equation of motion, with respect to ψ_1 , the matrix element over the vacuum state, and, taking into account constraint (25), we get

$$C(\mathbf{r}, t) = 0 .$$

The latter equation results in the Lagrange multiplier (54), which yields $H^{(1)} = 0$. Thus, in order to preserve constraint (25), the linear terms in the Hamiltonian must be zero.

The physical meaning of the proved theorem, that $\langle \psi_1 \rangle = 0$ necessarily requires $H^{(1)} = 0$, is quite evident. The terms in the Hamiltonian, linear in ψ_1 and ψ_1^\dagger describe the physical processes of annihilation and creation of single particles. If such processes were permitted, then the function $C(\mathbf{r}, t)$, introduced above, is not zero. Then the evolution equation for the average $\langle \psi_1(\mathbf{r}, t) \rangle$ contains the term

$$\int_0^t C(\mathbf{r}, t') dt'$$

generating the nonzero value of $\langle \psi_1 \rangle$.

One should not confuse the considered situation with the often used method of specially adding to the Hamiltonian the terms, linear in ψ_1 and ψ_1^\dagger , in order to break the gauge symmetry. Then, of course, the average $\langle \psi_1 \rangle$ is not zero. But at the end of calculations, one always set the additional linear terms to become zero, hence restoring the property $\langle \psi_1 \rangle = 0$. This procedure is what is called the Bogolubov method of infinitesimal sources [3,4]. These sources are usually lifted after the thermodynamic limit, but can also be made infinitesimally small in the process of taking the thermodynamic limit, provided this is done in the appropriate way [5,66]. In the approach, followed in the present paper, we do not need to introduce infinitesimal sources, since the gauge symmetry has already been broken by the Bogolubov shift (16).

Appendix C

The critical temperature T_c for the Bose system with contact interactions has been obtained, in the HFB approximation, from expansions for the condensate fraction (149) and superfluid fraction (150). This temperature was found to coincide with the critical temperature of the ideal Bose gas. In order to emphasize the correctness of this result, let us consider, first, the more general case of an arbitrary interaction potential $\Phi(\mathbf{r})$, provided it possesses the standard property of symmetry, such that $\Phi(-\mathbf{r}) = \Phi(\mathbf{r})$, and diminishes sufficiently fast with increasing $|\mathbf{r}|$.

At the critical temperature T_c , when $\rho_0 = 0$ and $\rho_1 = \rho$, Eq. (112) reduces to

$$\omega_k = \frac{k^2}{2m} + \frac{1}{V} \sum_p n_p (\Phi_{k+p} - \Phi_p) .$$

The Fourier transform

$$\Phi_{k+p} = \int \Phi(\mathbf{r}) e^{-i(\mathbf{k}+\mathbf{p})\cdot\mathbf{r}} d\mathbf{r}$$

can be simplified remembering that, by assumption, the interaction potential diminishes fast with increasing $r \equiv |\mathbf{r}|$. Then in the above integral, one can expand $e^{-i\mathbf{k}\cdot\mathbf{r}}$ in powers of $\mathbf{k} \cdot \mathbf{r}$ up to the second order. As a result, we get

$$\Phi_{k+p} \cong \left(1 - \frac{1}{6} k^2 r_0^2\right) \Phi_p ,$$

where the notation for the effective interaction radius r_0 is introduced, defined by the equation

$$r_0^2 \equiv \frac{\int r^2 \Phi(\mathbf{r}) d\mathbf{r}}{\int \Phi(\mathbf{r}) d\mathbf{r}} .$$

In this way, we find

$$\omega_k = \frac{k^2}{2m} - \frac{1}{6V} \sum_p n_p \Phi_p k^2 r_0^2 .$$

The critical temperature is given by the equation

$$\rho = \int n_k \frac{d\mathbf{k}}{(2\pi)^3} ,$$

in which

$$n_k = \left(e^{\omega_k/T_c} - 1\right)^{-1} .$$

From here we obtain

$$T_c = \frac{2\pi}{m^*} \left[\frac{\rho}{\zeta(3/2)} \right]^{2/3} ,$$

where the effective mass is

$$m^* \equiv \frac{m}{1 - \frac{m r_0^2}{3} \int n_k \Phi_k \frac{d\mathbf{k}}{(2\pi)^3}} .$$

Thus, for nonlocal interactions, with an interaction radius r_0 , the effective mass increases, so that the critical temperature diminishes, as compared to the critical temperature of the ideal Bose gas.

However, for the contact interaction potential (83), we have $r_0 = 0$, hence $m^* = m$, and T_c , in the frame of the HFB mean-field approximation, coincides with the ideal gas condensation temperature.

This conclusion is in agreement with other studies of the critical temperature for interacting Bose gas. There exists quite a number of such investigations, as reviewed in Refs. [31,49]. The most accurate of these calculations are those employing Monte Carlo simulations [67–71] and those based on the optimized perturbation theory [72–74], as has been done in Refs. [75–80]. These investigations show that the first correction to the critical temperature comes from effects beyond the mean-field approximation.

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